The Beilstein™ Commander

Application - CrossFire

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INFORMATION

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Manual: Version 2, September 1996, for Beilstein Commander Version 2.1 and CrossFire Server Version 3.1

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1

1. The Commander

The Beilstein Commander provides the user interface for Beilstein´s suite of products. Since the different products, for example CrossFire and Autonom, have different interface requirements, the Commander configures itself accordingly.

When using CrossFire, the Commander is configured with a Structure and Reaction editor, a Fact editor, and the Display Hits module. These are all linked together through the Commander to give one coherent interface unit.

The Commander provides the means to access the CrossFire, and your own customer databases; allowing searches to be carried out, results displayed and the database to be browsed - thus giving you the ability to navigate seamlessly through the world of organic chemistry.

1.1 System Requirements (recommended)

	IBM PC or compatible	**Macintosh**
Platform	486 PC compatible, or Pentium PC	68040 class computer, or PowerPC chip class computer
Memory	12 Mbyte not including OS requirements	16 Mbyte not including OS requirements
Storage	15 Mbyte hard disk storage	15 Mbyte hard disk storage
Operating System	MS Windows 3.1x MS Windows NT, or MS Windows 95	Mac OS 7.5 Release 2
Connectivity	MS Winsocket 1.1 compliant	Mac TCP
Protocol	TCP/IP connection to server (Novell LAN Workplace 4.0/4.1 or TCP/IP extension products that are Winsocket 1.1 compliant)	TCP/IP connection to server

1.2 Windows Set-up

The set-up procedure describes the installation of the client software only. For information concerning the server, please consult the server guide.

Before you start the setup procedure, we recommend that you prepare a backup copy of your set of installation disks.

The Setup can be stopped at any time by clicking the ‘Cancel’ button. You will also be able to navigate through the dialog boxes of Setup by using the ‘Next’ and ‘Back’ buttons until copying of the files starts.

1.2.1 Start

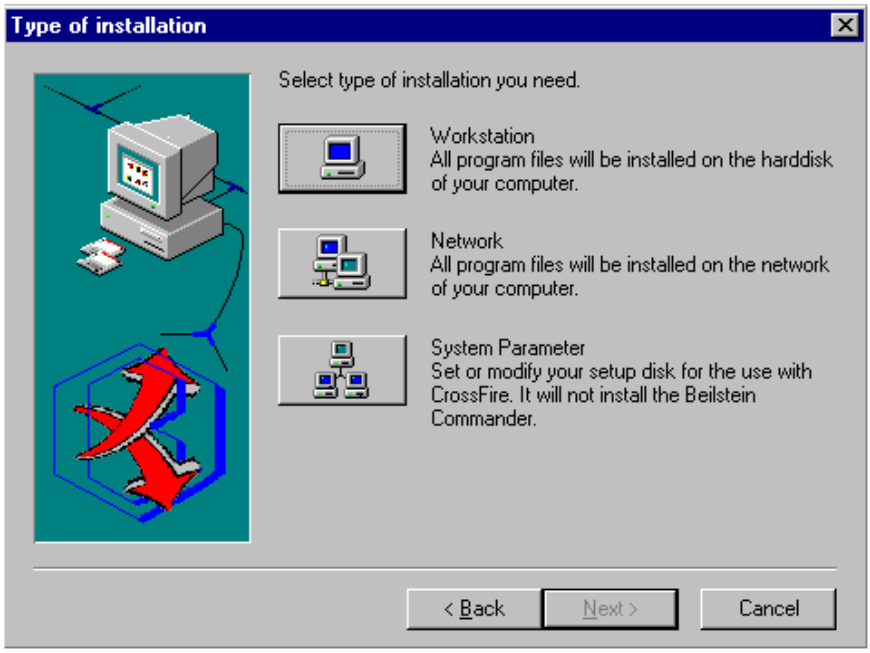
On starting SETUP.EXE the following dialog box will appear:

Setup
Beilstein Commander - Application CrossFire for Windows 95
Welcome
Welcome to the Beilstein Commander Setup program. This program will install Beilstein Commander on your computer.
It is strongly recommended that you exit all Windows programs before running this Setup program.
Click Cancel to quit Setup and then close any programs you have running. Click Next to continue with the Setup program.
WARNING: This program is protected by copyright law and international treaties.
Unauthorized reproduction or distribution of this program, or any portion of it, may result in severe civil and criminal penalties, and will be prosecuted to the maximum extent possible under law.
Next >
Cancel

Setup automatically recognizes the operating system and will install the appropriate Beilstein Commander version. The headline tells you the version that will be installed (in the above example: Windows95).

Choose ‘Next’ to proceed with the installation or ‘Cancel’ to exit the setup.

1.2.2 Type of Installation

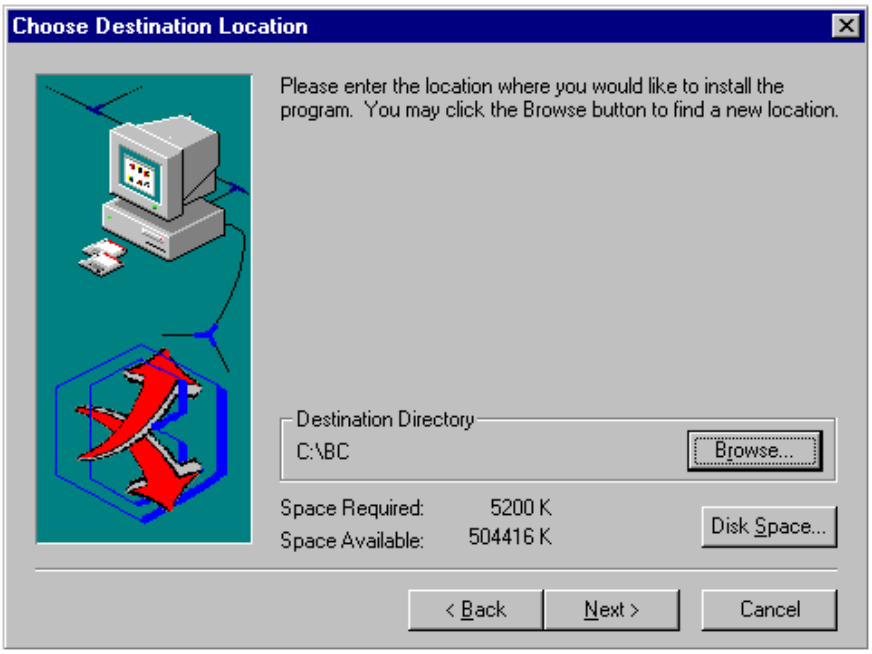

Type of installation
Select type of installation you need.
Workstation
All program files will be installed on the harddisk of your computer.
Network
All program files will be installed on the network of your computer.
System Parameter
Set or modify your setup disk for the use with CrossFire. It will not install the Beilstein Commander.
< Back
Next >
Cancel

Choose ‘Workstation’ to install the Commander on a single PC.

Choose ‘Network’ to install the Commander program files on a network server together with a setup for user workstations. This setup is a modified version of the disk setup; if a user launches this setup, he only needs to enter a path for his local working directory and a name for the program group. All other settings will be taken from the network installation. The modified setup will only copy some system files into the local Windows installation of the user. It will not copy any Beilstein Commander files to the user directory.

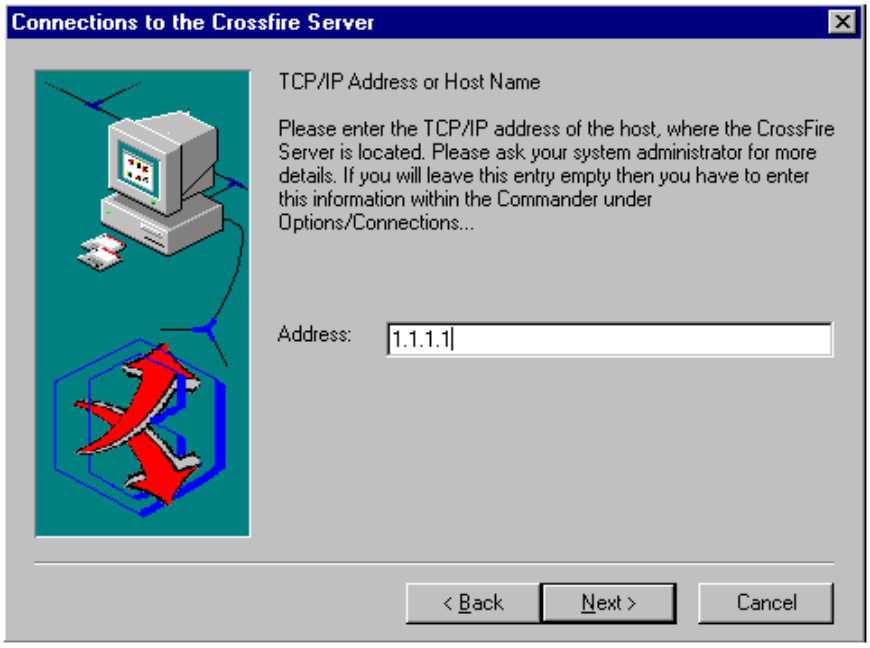
Choose ‘System Parameter’ if you want to define system settings for use with the CrossFire server and to modify the first setup diskette. After this has been completed, Setup will exit without installing the Beilstein Commander . You can now distribute the set of installation diskettes among other users of the system. If they run the setup again from the modified diskettes, they will not see the System Parameter option, and they will not be prompted for any CrossFire system parameter settings. Remember to use a backup copy of the installation diskettes before you choose this option!

1.2.3 The Destination Path


Choose Destination Location
Please enter the location where you would like to install the program. You may click the Browse button to find a new location.
Destination Directory
C:\BC
Browse...
Space Required: 5200 K
Space Available: 504416 K
Disk Space...
< Back
Next >
Cancel

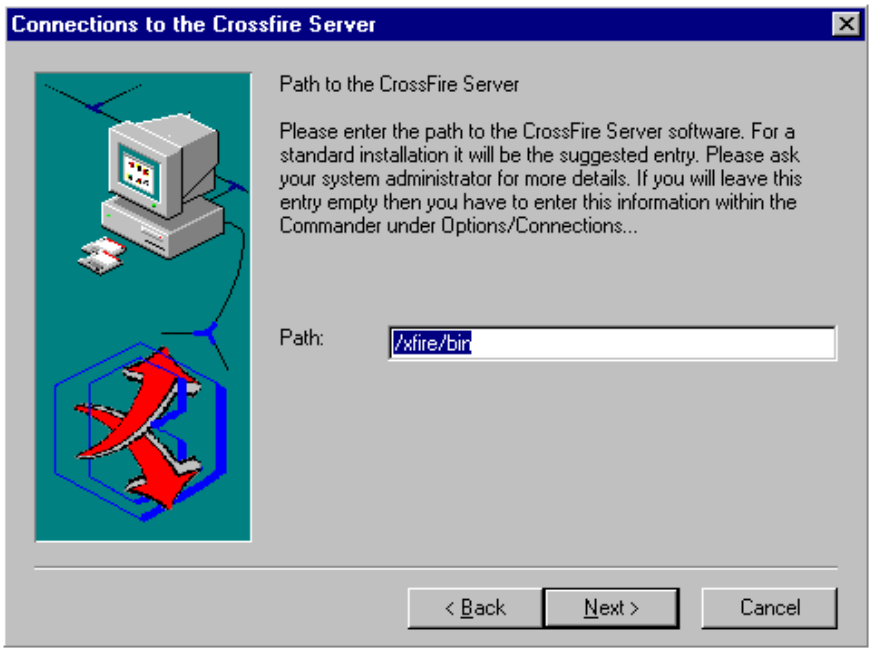
Click the ‘Browse’ button to select, or enter the complete path of the directory in which the program and associated files should be installed. Make sure that you have write access for the directory. The button ‘Disk Space’ allows you to select a drive.

1.2.4 The CrossFire Host Address


Connections to the Crossfire Server
TCP/IP Address or Host Name
Please enter the TCP/IP address of the host, where the CrossFire Server is located. Please ask your system administrator for more details. If you will leave this entry empty then you have to enter this information within the Commander under Options/Connections...
Address:
1.1.1.1
< Back
Next >
Cancel

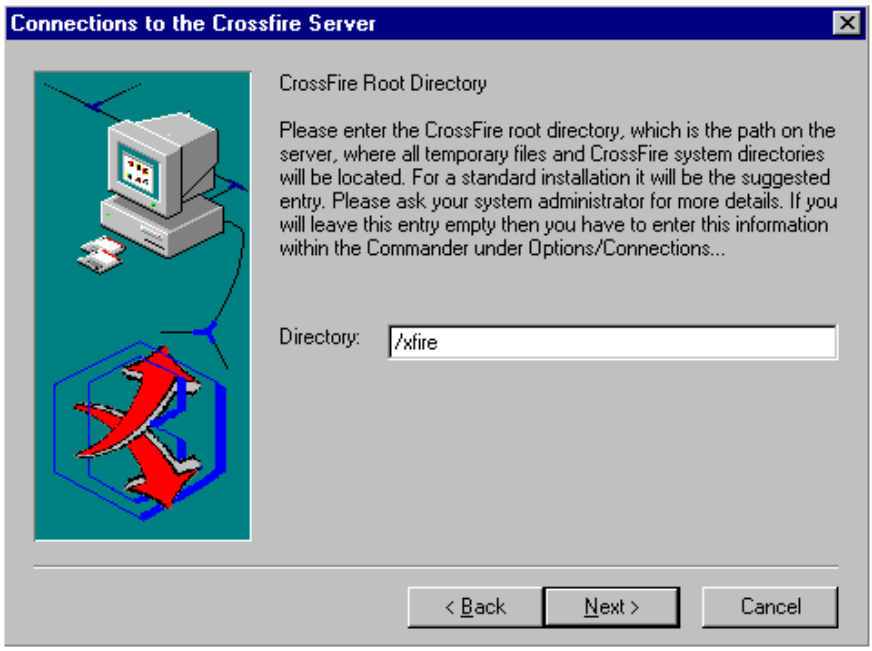
Enter the TCP/IP address of the host where the CrossFire server is located. Please ask your system administrator for more details. You can skip this and enter the information later in the Communications dialog box which is in the options menu of the Commander.

1.2.5 CrossFire Server Path


Connections to the Crossfire Server
Path to the CrossFire Server
Please enter the path to the CrossFire Server software. For a standard installation it will be the suggested entry. Please ask your system administrator for more details. If you will leave this entry empty then you have to enter this information within the Commander under Options/Connections...
Path:
/xfire/bin
< Back
Next >
Cancel

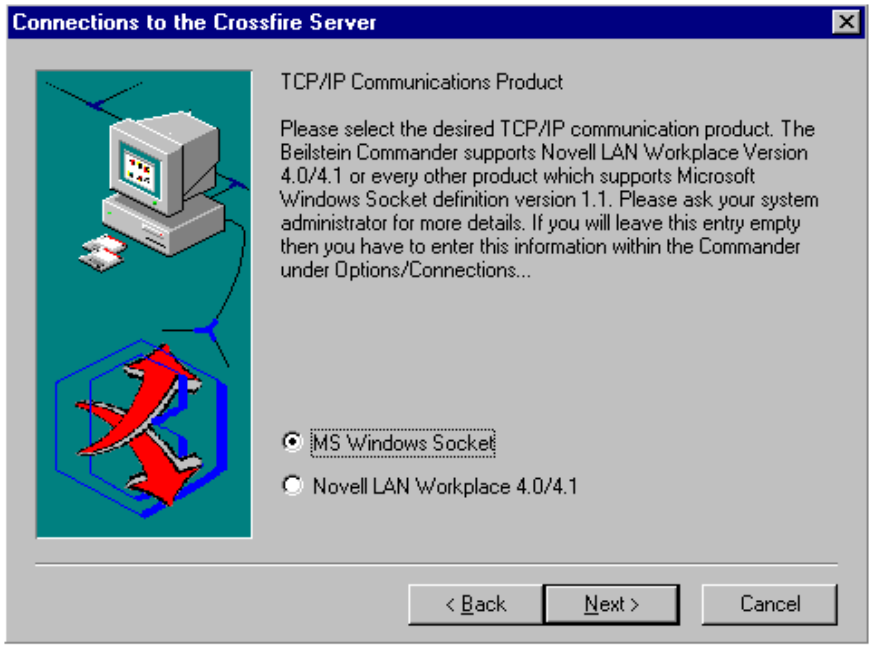
Enter the path to the CrossFire server. The suggested entry corresponds to a standard installation. Please ask your system administrator for more details. You can skip this and enter the information later in the Communications dialog box which is in the options menu of the Commander.

1.2.6 CrossFire Root Directory


Connections to the Crossfire Server
CrossFire Root Directory
Please enter the CrossFire root directory, which is the path on the server, where all temporary files and CrossFire system directories will be located. For a standard installation it will be the suggested entry. Please ask your system administrator for more details. If you will leave this entry empty then you have to enter this information within the Commander under Options/Connections...
Directory:
/xfire
< Back
Next >
Cancel

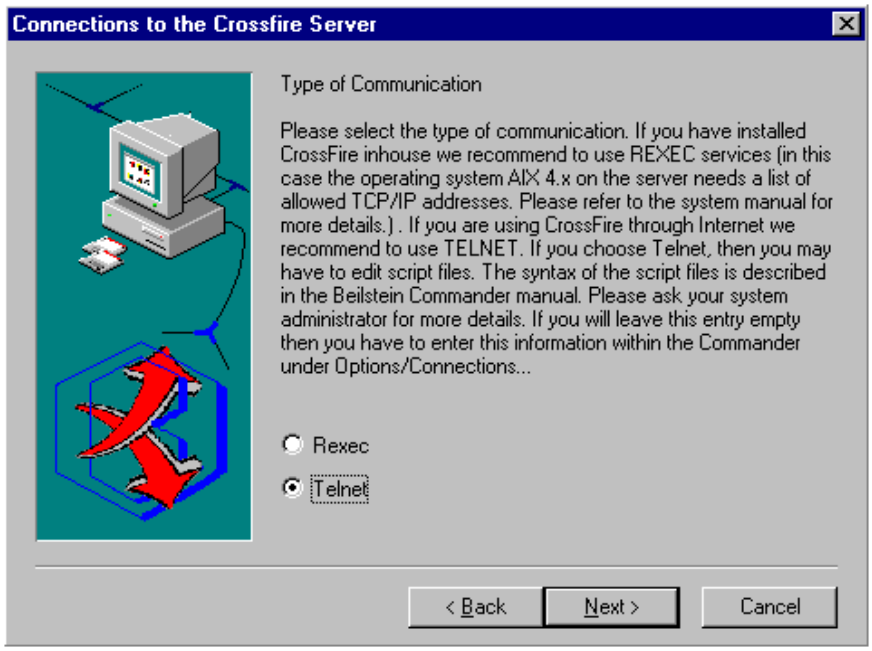
Enter the CrossFire root directory. The suggested entry corresponds to a standard installation. Please ask your system administrator for more details. You can skip this and enter the information later in the Communications dialog box which is in the options menu of the Commander.

1.2.7 TCP/IP Communications Product


Connections to the Crossfire Server
TCP/IP Communications Product
Please select the desired TCP/IP communication product. The Beilstein Commander supports Novell LAN Workplace Version 4.0/4.1 or every other product which supports Microsoft Windows Socket definition version 1.1. Please ask your system administrator for more details. If you will leave this entry empty then you have to enter this information within the Commander under Options/Connections...
MS Windows Socket
Novell LAN Workplace 4.0/4.1
< Back
Next >
Cancel

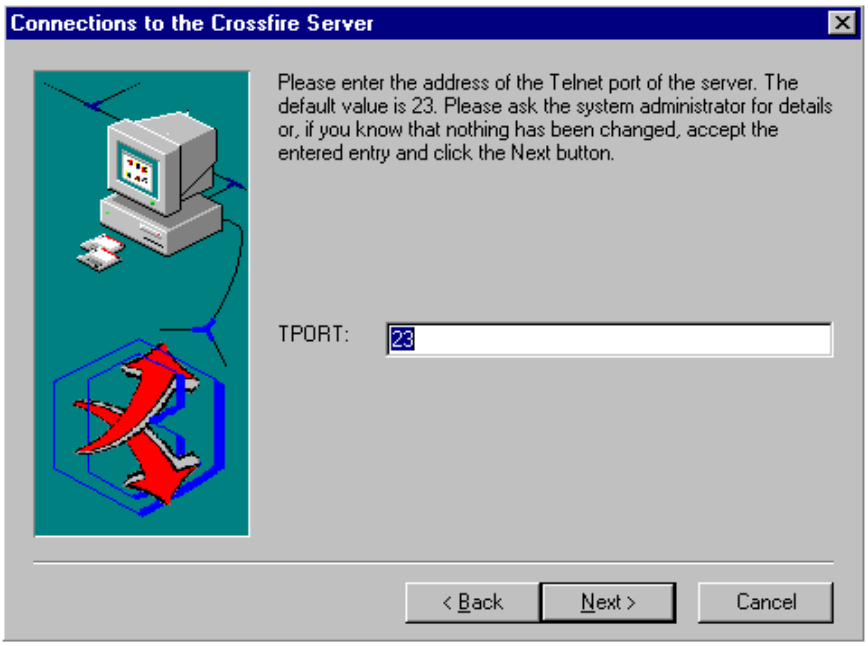
Enter the desired TCP/IP communications product. The Beilstein Commander supports Novell LAN Workplace version 4.0/4.1 or other products that support the Microsoft Windows Socket TCP/IP definition version 1.1. Please ask your system administrator for more details. You can skip this and enter the information later in the Communications dialog box which is in the options menu of the Commander.

1.2.8 Type of Communication


Connections to the Crossfire Server
Type of Communication
Please select the type of communication. If you have installed CrossFire inhouse we recommend to use REXEC services (in this case the operating system AIX 4.x on the server needs a list of allowed TCP/IP addresses. Please refer to the system manual for more details.) . If you are using CrossFire through Internet we recommend to use TELNET. If you choose Telnet, then you may have to edit script files. The syntax of the script files is described in the Beilstein Commander manual. Please ask your system administrator for more details. If you will leave this entry empty then you have to enter this information within the Commander under Options/Connections...
Rexec
Telnet
< Back
Next >
Cancel

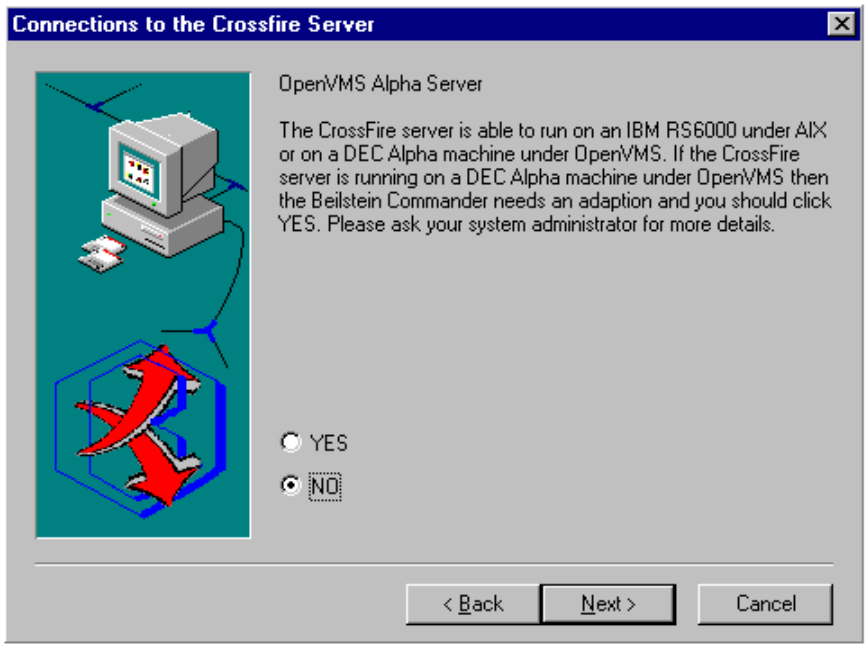
Enter the type of communication. If you have CrossFire installed in-house, then we recommend that you use REXEC services. If you are using CrossFire through Internet, then we recommend Telnet. If you choose Telnet then you may have to edit script files. They will be available through the Beilstein Commander under Options/Communications. Please refer to the appendix of the Beilstein Commander guide or to chapter 3 of this guide for a description of the script syntax. Please ask your system administrator for more details. You can skip this and enter the information later in the Communications dialog box which is in the options menu of the Commander.

1.2.9 Type of Communication - Port Settings


Connections to the Crossfire Server
Please enter the address of the Telnet port of the server. The default value is 23. Please ask the system administrator for details or, if you know that nothing has been changed, accept the entered entry and click the Next button.
TPORT:
23
< Back
Next >
Cancel

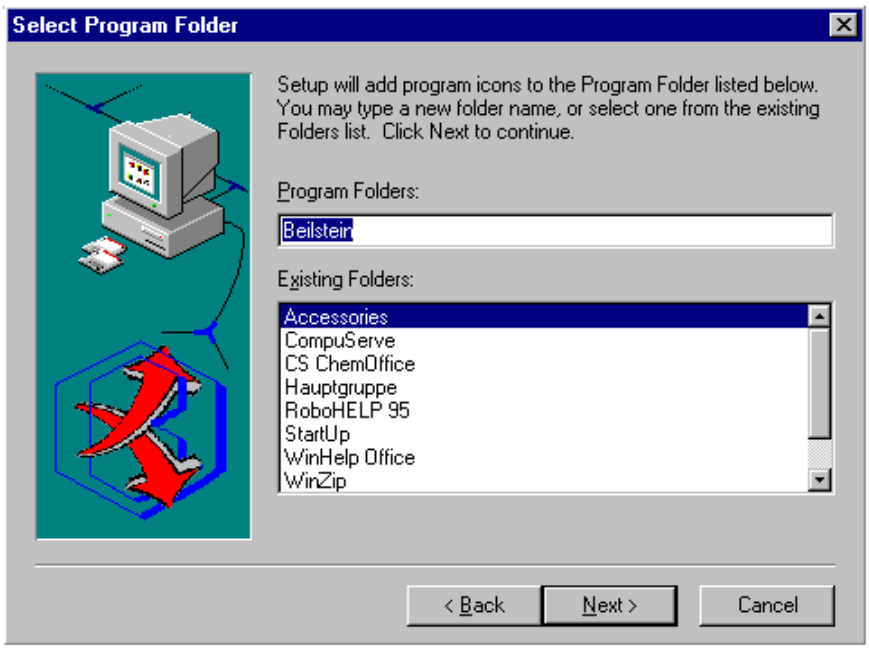
Telnet and Rexec port numbers (TPORT and/or RPORT) can be set on the server by the system administrator. The default value for the TPORT is 23 and for the RPORT 512. If you see a ”greyed-out” entry you should accept the setting as is, and click on the ‘Next’ button. For more details please contact your system administrator.

1.2.10 OpenVMS Alpha Server


Connections to the Crossfire Server
OpenVMS Alpha Server
The CrossFire server is able to run on an IBM RS6000 under AIX or on a DEC Alpha machine under OpenVMS. If the CrossFire server is running on a DEC Alpha machine under OpenVMS then the Beilstein Commander needs an adaption and you should click YES. Please ask your system administrator for more details.
YES
NO
< Back
Next >
Cancel

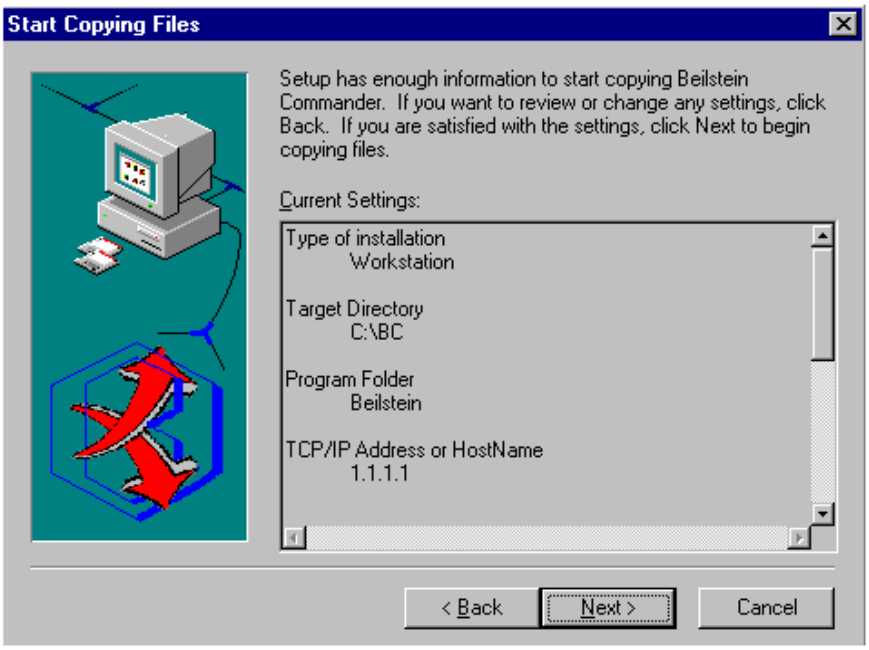
The CrossFire server is also available for DEC Alpha machines running under OpenVMS 6.2 or higher. If you have CrossFire installed on A DEC Alpha, you should select YES. Please ask your system administrator for details.

1.2.11 Program Group Selection



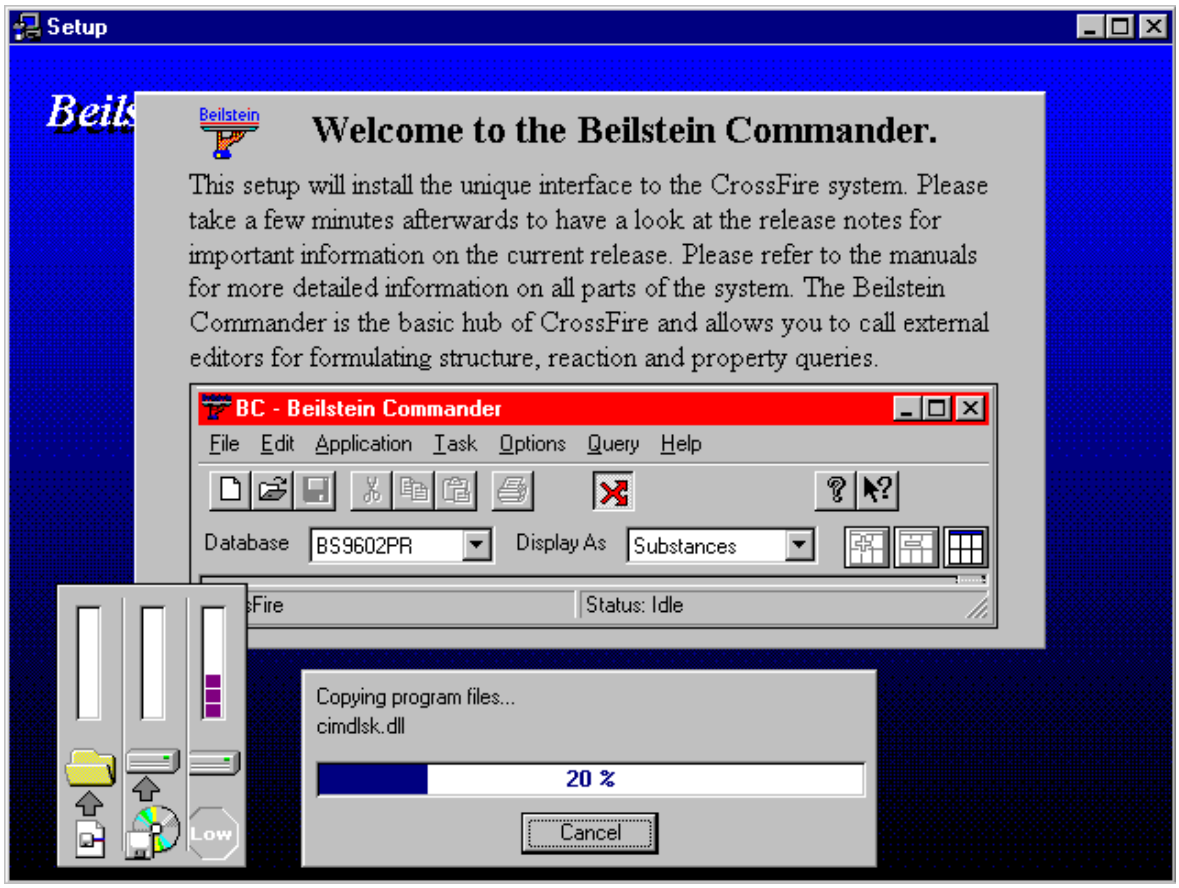
Please enter or select a name of the Program Group where you would like to have the Beilstein Commander icon installed on your desktop. The default value is ‘Beilstein’.

1.2.12 Installation Parameters Summary


Start Copying Files
Setup has enough information to start copying Beilstein Commander. If you want to review or change any settings, click Back. If you are satisfied with the settings, click Next to begin copying files.
Current Settings:
Type of installation
Workstation
Target Directory
C:\BC
Program Folder
Beilstein
TCP/IP Address or HostName
1.1.1.1
< Back
Next >
Cancel

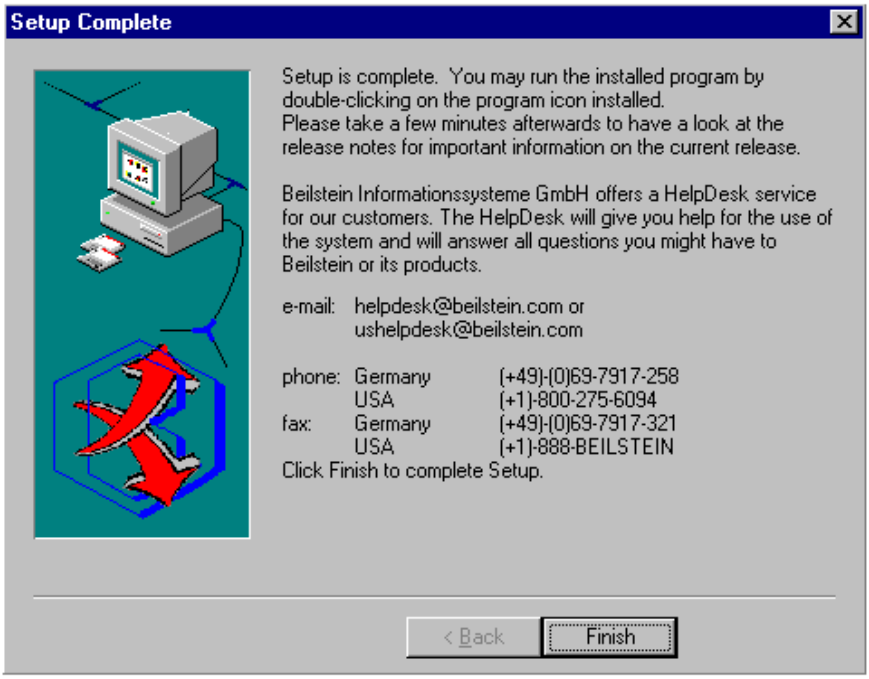
Before the installation starts, Setup will give you an overview of all parameters entered so far. At this point you can to go back and change some settings. If you click on ‘Next’ the installation will proceed.

1.2.13 Installation Process Indicator


Setup
Welcome to the Beilstein Commander.
This setup will install the unique interface to the CrossFire system. Please take a few minutes afterwards to have a look at the release notes for important information on the current release. Please refer to the manuals for more detailed information on all parts of the system. The Beilstein Commander is the basic hub of CrossFire and allows you to call external editors for formulating structure, reaction and property queries.
BC - Beilstein Commander
File Edit Application Task Options Query Help
Database BS9602PR
Display As Substances
Status: Idle
Copying program files...
cimdlsk.dll
20 %
Cancel
Low

At this point you will be shown several graphics containing previews of the new Beilstein Commander, some dialog boxes about the progress of the installation.

1.2.14 Finished


Setup Complete
Setup is complete. You may run the installed program by double-clicking on the program icon installed.
Please take a few minutes afterwards to have a look at the release notes for important information on the current release.
Beilstein Informationssysteme GmbH offers a HelpDesk service for our customers. The HelpDesk will give you help for the use of the system and will answer all questions you might have to Beilstein or its products.
e-mail: helpdesk@beilstein.com or
ushelpdesk@beilstein.com
phone: Germany (+49)-(0)69-7917-258
USA (+1)-800-275-6094
fax: Germany (+49)-(0)69-7917-321
USA (+1)-888-BEILSTEIN
Click Finish to complete Setup.
< Back
Finish

The final dialog box tells you whether the installation has succeeded or not. Click ‘Finish’ to finish the setup procedure.

After a successful installation, you can start the Commander by double-clicking the

icon in the Program Manager.

1.3 Macintosh Setup

Start the Beilstein Commander Installer by double-clicking the icon.

This installer will place the Beilstein Commander software in a folder called Beilstein on your hard disk.

The installer will automatically recognize the processor on the Macintosh, and will install only the version of the Beilstein Commander appropriate for your Macintosh, e.g. the native Power Macintosh version for a Power Macintosh and the native 68K Macintosh version for machines with a 68xxx processor.

If you have an older version of the Beilstein Commander already installed, the installer will ask you to “OK” deleting old preference files. You should accept this.

The installer will also install a folder containing a complete MacTCP installation package. The Beilstein Commander needs a MacTCP compliant TCP/IP communication product to get access to the CrossFire server. If you don’t have MacTCP on your machine, then you may use the tools included with the Beilstein Commander install. Please ask your system administrator or the Beilstein HelpDesk for details.

After the installation you need to know a few things to get CrossFire running:

- the TCP/IP address of the server,
- the CrossFire directories on the server.

You have to enter this information within the Beilstein Commander under Options/Connections. Please, contact your system administrator for details.

If your environment is using a firewall, then you have to edit a script file.

Please take a look at the manuals for detailed information.

In addition you need to know your

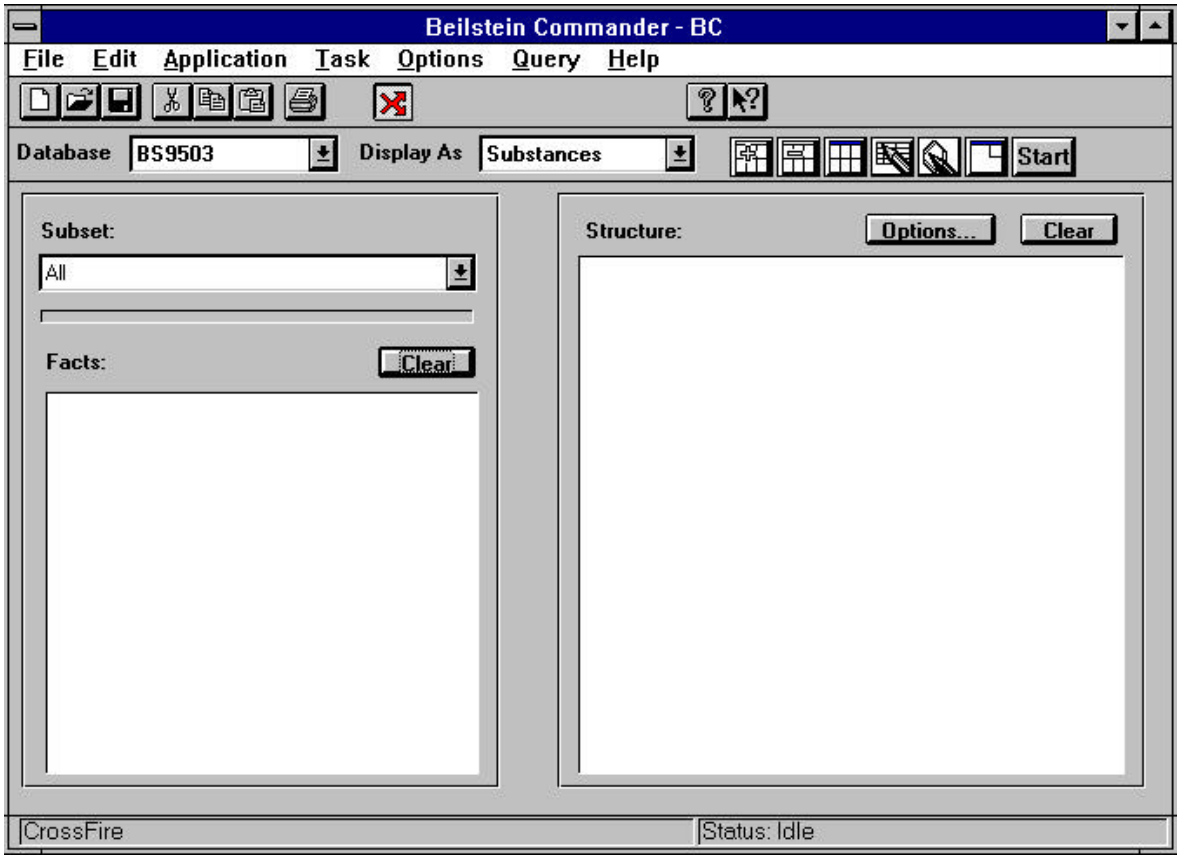
- User-Id and
- Password.

The system will ask you for that if you try to connect to the server. Please, ask your system administrator for this information.

1.4 Working with the Beilstein Commander

The Commander interface is configured automatically, according to the application selected.

The buttons in the APPLICATION FUNCTION BAR and the options in the application menu will be activated according to the applications that you have installed.



Once installed, the unchanging features of the Commander consist of a Menu Bar, Status bar, and the Application Function Bar (see below).

Depending on the application, the TASK FUNCTION BAR and both the structure and facts panels are configured and displayed appropriately.

When the user switches from one application to another, the contents of the Structure window and Facts window remain constant. When the user selects a different application, which causes a panel to disappear, it would be made invisible but would be re-displayed, including contents, on selection of the original application.

1.4.1 The Application Function Bar

The APPLICATION FUNCTION BAR has (assuming the maximum number of products) the following controls:

A series of standard Windows interface buttons: new, open, save, print, copy, paste etc.

Buttons to select the current application; you may choose from:

CrossFire or Autonom (if it is installed)

Pressing the button for an application switches to the relevant Commander mode for that application, but does not start a search or Autonom etc.

See the appendix for a description of the applications.

CrossFire plusReactions

2

2. *CrossFire* plus*Reactions*

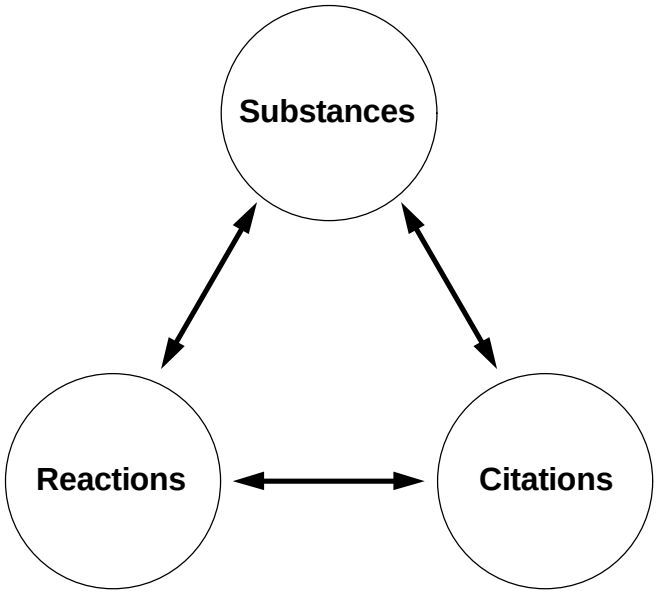
CrossFire *plus*Reactions is a complete chemical information system comprised of the Beilstein Database, the CrossFire search and retrieval server software, and the Beilstein Commander client. The Beilstein Commander runs under Microsoft Windows or on an Apple Macintosh.

2.1 System Design

2.2 Searching

2.1 System Design

CrossFire *plus*Reactions provides a new approach to handling chemical information. The emphasis is on content, not on form. There are no artificial barriers between the different ways of viewing information, CrossFire allows you to search and display chemical information the way you want, whether it is in terms of Substances (Structures and Properties), Reactions, or Citations, and provides hyperlinks between the different data domains.



Substances. The database contains over 30 million reports on properties of about 7 million organic compounds. You can access the structures and their associated chemical, physical, physiological and bibliographic information. Hyperlinks are available to reactions and literature references, as well as to other referenced compounds such as precursors or components.

Reactions. The database contains over 5 million reactions which are searchable, with CrossFire *plus*Reactions, as reaction substructures. You can define the role of a structure or substructure in the reaction, and search using reaction attributes such as reaction centers, bond fate and atom-atom mapping. Hyperlinks allow navigation to Substances and to Literature references.

Citations. These are now stored in a separate domain of the database. This facilitates citation searching and a citation orientated display. You can now display, in one document, all of the compounds and reactions that have been abstracted from the original reference. Hyperlinks, again, are provided to Substances and Reactions.

Hyperlinks. These allow seamless navigation between substances, reactions and citations. Thus, for example, when you are viewing a reaction, one mouse click on the hyperlink calls up the substance record for one of the reaction partners. Similarly when viewing some properties, simply click on the citation hyperlink to call up the citation record showing all the compounds and reactions abstracted from that reference.

Display Context. You can carry out structure searches (on the whole database or on subsets), factual searches and combined searches. The Display Context of the search, which is automatically set at search time (a search for reactions will result in a display in reaction context), can be subsequently changed for either single compounds, lists of compounds (or reactions or citations) or for the whole hit set.

By using combinations of searches, changes of context and hyperlinks, navigation through the database results not only in solutions to organic chemistry problems, but by acting as a creativity enhancer, it may lead to serendipitous discoveries.

2.2 Searching

With CrossFire *plus*Reactions you can search for Structures, Reactions, Properties and other factual information.

Structures: Full structures, substructures, generic structures, stereoisomers and tautomers can be searched for. You can use global query options such as ”Free Sites on All Atoms“, or set options on specific atoms and bonds only. Query atom types such as ”X“ (any halogen) can be set, as can Atom lists (e.g. A1= C, N, O, S). Predefined generic groups, e.g. ALK (alkyl), and user defined generic groups (Markush structures) are easily input.

Reactions: All the features availble in structures, *plus* reaction role (reactant or product), reaction center, bond fate and atom-atom mapping.

Thus you can search for half reactions of the type:

? => A "how do I make this type of compound"

A => ? "what do these starting materials give"

or full reactions of the type:

A => B "general or specific transformations".

Properties: search for numeric values and ranges, strings, and keywords. The CrossFire database contains more than 30 million reports on chemical, physical, and physiological properties. You can search, for example, for chemical name, reaction conditions, biological function. All of these are stored in discrete fields. See the reference guide for more information.

3

3. The CrossFire Interface

3.1 The Task Function Bar

3.2 Structure/Reaction Panel

3.3 ***Facts*** Panel

3.4 Subset Selection Box

3.5 Combined Queries Operator

3.1 The Task Function Bar

The TASK FUNCTION BAR features combo boxes and buttons that are configured according to the active application. For a detailed explanation see the sections about the Query menu and the Task menu

The task function bar has the following controls:

The Database Selection Box allows you to choose between Beilstein databases and any Customer's CrossFire Structure and Reaction databases.

The Display Context Box. Choose to display context from: Substance, Reaction or Citation. This box will only be enabled when the Beilstein File has been selected in the database combo box.

The Database Browse Button . Pressing the button starts the browser which allows you to browse through the selected database. The database can be browsed and structures copied to the Commander.

The Update Database Button . This button will only be visible and enabled when a customer database has been selected in the database combo box. Pressing the button starts the browser - *in update mode*. The database can be browsed, and structures present in the Commander can either be added as new records to the database, or it can overwrite existing records.

Delete Database Record . This button will only be enabled when a customer database has been selected in the database combo box. Pressing the button starts the browser - *in delete mode*. The database can be browsed and the selected structure can be deleted.

Fact Editor. Pressing this button will start the Fact Editor.

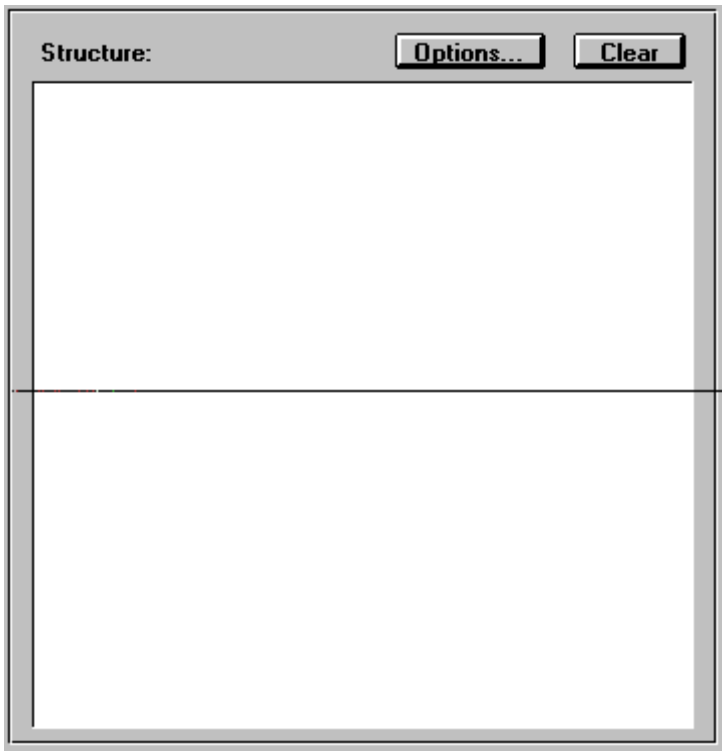
Structure Editor Pressing this button will start the Structure Editor.

Display. This button will only be active if a hitset has been created. Pressing this button will switch to Display.

Start. This button will only be active if a fact query or structure is present. Press the button to start the CrossFire application.

3.2 Structure/Reaction Panel

The structure panel has three controls; the Structure Window, the structure query options button and a clear button.



3.2.1 Structure Window

The structure editor can be activated by double clicking the window.

Pressing the clear button deletes the contents of the structure and query options windows.

⌘ Windows

The structure editor to be used will be that set in the preferences menu.

Beilstein Structure Editor . If query options have been set, on returning to the Commander, the options will be displayed as a string in the structure window.

Non-Beilstein Structure Editor . On returning to the Commander, the structure will have been converted to a Rosdal string for display in the structure window. If some attributes could not be converted, a message to that effect will be displayed in a message box. Please take a look at the appendix for a description of the limitations.

Setting Structure Query Options . Since these cannot be set from within the Non-Beilstein Structure Editor, they must be set in the Commander. Pressing the Options button causes the query option dialog box to be displayed. The options

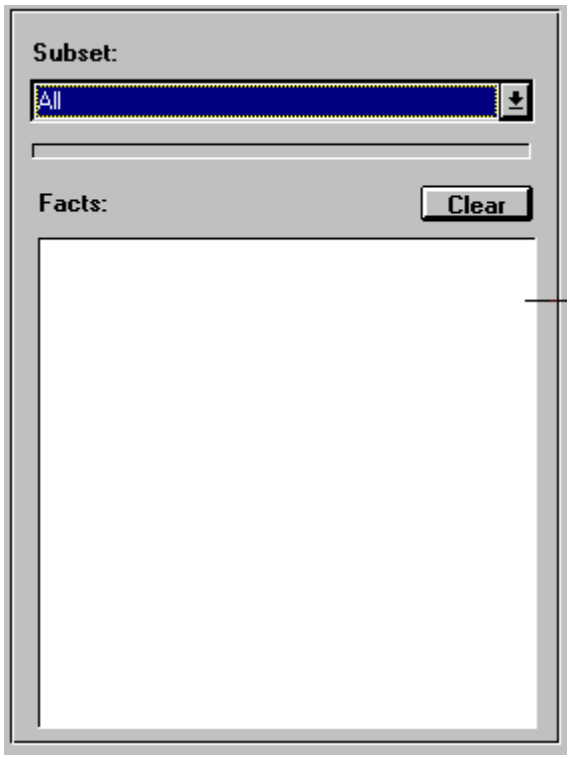
can then be set and when the box is closed they will be displayed as a string in the options window.

⌘ Macintosh

With this version of the Beilstein Commander, the Beilstein structure editor is the one available for Apple Macintosh users.

3.3 Facts Panel

The Facts panel has three controls: the Facts Window , the Subset Selection Box and the clear button.



3.3.1 Facts Window

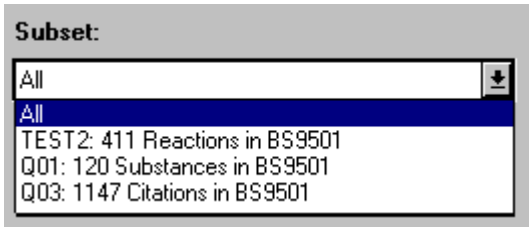
Double clicking the FACTS window switches to the Fact Editor. All factual queries are input here, as well as combined queries with other facts or hit lists (including those from structures or reactions). After switching back to the Commander, the query string is displayed in the Facts window.

Pressing the clear button deletes the contents of the window.

3.4 Subset Selection Box

The subset window provides a quick means of selecting a previous hit set for further use, either in combination with a structure query or for a change of context. The default is ”All“ signifying the complete database. The hit set can also be selected in the Fact Editor.

Thus, the combo box will contain a list of all permanently saved hit lists and all session hit lists, displayed as follows:



When the subset is selected, it will overwrite the present (if any) factual query.

3.5 Combined Queries Operator

When a combined query has been input in the Commander with entries in both the Facts panel and the Structure panel, the combined queries operator will be displayed as a label between the two panels **. The setting is always AND** . When one of the panels is cleared the label will not longer be displayed.

The fact query will always be searched for first, and the resulting hitset will be used as a subset for the structure search.

4

4. The CrossFire Menu Options

The Menu bar has the following options:

4.1 File menu

4.2 Edit menu

4.3 Application menu

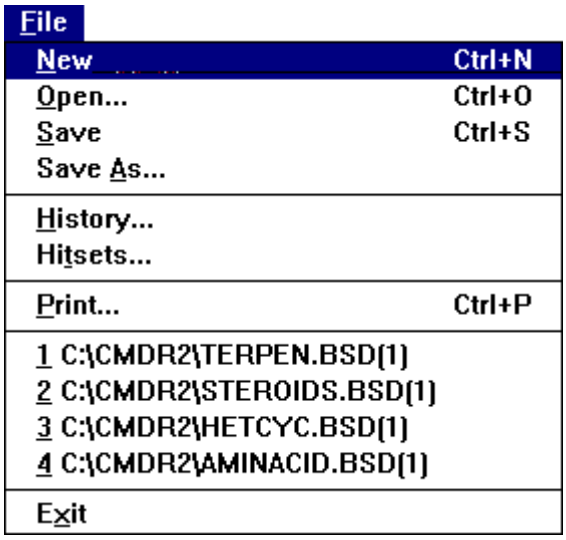
4.4 Task menu

4.5 Options menu

4.6 Query menu

4.1 File menu commands

The File menu has the following options(Windows version is shown):



4.1.1 New

Use this command to create a new document in the Beilstein Commander.

You can open an existing document with the Open command.

Shortcuts

Toolbar:

Keys: CTRL+N

Macintosh **⌘ N** **Command N**

4.1.2 Open command

Use this option to load previously stored queries into the Commander. When you choose this option, the File Open dialog box will be displayed, where you can select the file you want to open.

You can create new documents with the New command.

Shortcuts

Toolbar:

Keys: CTRL+O

Macintosh **⌘ O** **Command O**

1. Choose Open from the file menu to display the File Open dialog box. This box allows selection of the drive, path, and file to be opened.

2. Select a file. If you know which query you want to load, enter the number in the INO field and click OK. If you would like to examine the contents of the file click the browse button to start the Browser.

3. Browse through the contents either using the slider or the page keys to view the file. You can start browsing at a particular query by entering its number in the INO field.

4. Double click a query, or choose "Load Entry" from the file menu to transfer the query to the Commander.

4.1.3 Save command

Use this command to save the active document to its current name and directory. When you save a document for the first time, the Beilstein Commander displays the Save As dialog box so you can name your document. If you want to change the name and directory of an existing document before you save it, choose the Save As command.

Shortcuts

Toolbar:

Keys: CTRL+S

Macintosh **⌘ S** **Command S**

Use this option to save queries in a file (*.bsd). First time use requires the input of a file name. Thereafter, when save is selected the fact query will be automatically stored in the same file under the same INO. Each file can contain more than one structure. Each structure is given an internal number (INO), starting with 1 for the first structure.

1. Choose Save from the file menu to display the file save dialog box.

Either

2. Input the internal number (INO) you want to assign to this query and click OK to store the query.

Or

3. Click the browse button to display the file contents. Either double click a cell to store the query, or select a cell and choose Save Entry from the File menu options.

To store a modified query under a different INO use Save As... .

4.1.4 Save As command

This option is similar to the save option except that it saves the query under a new file name or under a new INO in the same file.

To save a document with its existing name and directory, use the Save command.

1. Choose Save As... from the file menu to display the file save dialog box.

Either

2. Input the internal number (INO) you want to assign to this query and click OK to store the query.

Or

3. Click the browse button to display the file contents. Either double click a cell to store the query or select a cell and choose Save Entry from the File menu options.

4.1.5 …2, 3, 4 command

Use the numbers and filenames listed at the bottom of the File menu to open the last four documents you closed. Choose the number that corresponds with the document you want to open.

4.1.6 History

Select this option to call up the Browser to display the session History. You can load previous queries into the Commander by using the Load option in the Browser file menu.

4.1.7 Hitsets

This option starts the Browser, which displays the temporary session hitsets and any hitsets that you have permanently saved. You can load the query into the Commander by using the Load option in the File menu of the Browser.

4.1.8 Print command

Use this command to print a document. This command presents a Print dialog box, where you may specify printing either the actual query, or a range from the session queries, the number of copies, the destination printer, and other printer setup options.

Shortcuts

Toolbar:

Keys: CTRL+P

Macintosh ⌘ P **Command P**

4.1.9 Exit / Quit command

Use this command to end your Commander session. You can also use the Close command on the application Control menu. The Commander prompts you to save any queries or hitlists with unsaved changes.

Shortcuts

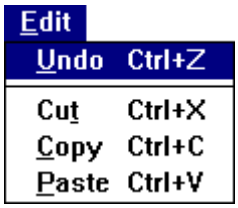
Mouse: Double-click the application's Control menu button.

Keys: ALT+F4

Macintosh ⌘ Q **Command Q**

4.2 Edit menu commands

The Edit menu has the following options (Windows version is shown):



4.2.1 Undo/Can't Undo command

Use this command to reverse the last editing action, if possible. The name of the command changes, depending on what the last action was. The Undo command changes to Can't Undo on the menu if you cannot reverse your last action.

Shortcuts

Keys: CTRL+Z or

ALT-BACKSPACE

Macintosh **⌘ Z** **Command Z**

4.2.2 Cut command

Use this command to remove the currently selected data from the document and put it on the clipboard. This command is unavailable if there is no data currently selected.

Cutting data to the clipboard replaces the contents previously stored there.

Shortcuts

Toolbar:

Keys: CTRL+X

Macintosh **⌘ X** **Command X**

4.2.3 Copy command

Use this command to copy selected data onto the clipboard. This command is unavailable if there is no data currently selected.

Copying data to the clipboard replaces the contents previously stored there.

Shortcuts

Toolbar:

Keys: CTRL+C

Macintosh **⌘ C** **Command C**

4.2.4 Paste command

Copies the contents of the clipboard to the active window. This will only be available if a section of text or a structure has been copied from the Hit Display to the clipboard.

Shortcuts

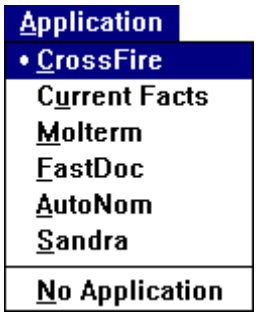
Toolbar:

Keys: CTRL+V

Macintosh **⌘ V** **Command V**

4.3 Application Menu Commands

The Application menu offers the following commands:



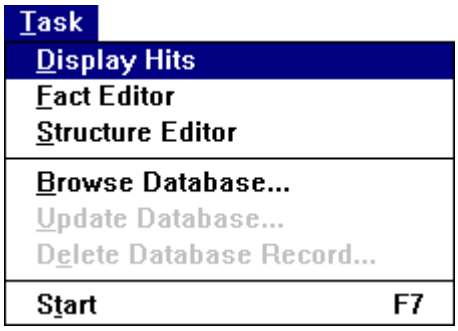
The individual applications are described in detail in the appendix.

4.3.1 Application No Application

Use this option to deactivate any application. This can be useful if, for example the communications link has broken down, and you need to start a new session. Simply select ”No application“ and then select the application that you would like to re-start.

4.4 Task menu commands

The Task menu offers the following commands:



4.4.1 Task Display

This option will only be available and enabled if a hit set has been created.

Select this option to switch to the display of search results.

More information about using the Display can be found in the Help for Display Hits or relevant manual section.

Button

4.4.2 Task Fact Editor

This option will only be enabled when CrossFire is the active application.

Selecting this option has the same effect as double-clicking the fact window and switches to the Fact Editor OLE server. The current query (if present) will be displayed in the editor.

More information about the operation of the Fact Editor can be found in the relevant manual section.

Button

4.4.3 Task Structure Editor

Selecting this option has the same effect as double-clicking the structure window and switches to the Structure Editor. The current query (if present) will be displayed in the editor.

More information about the operation of the Structure Editor can be found in the Structure Editor Help, or relevant manual section.

Button

4.4.4 Task Browse Database

Pressing the button starts the browser which allows you to browse through the selected database. The database can be browsed and structures copied to the Commander.

Button

4.4.5 Task Update Database

This option will only be available and enabled when a *customer database* has been selected in the database combo box.

Selecting this option starts the browser - **in update mode**. The database can be browsed and structures present in the Commander can either be added as new records to the database, or they can overwrite existing records.

Button

4.4.6 Task Delete Database Record

This option will only be available and enabled when a *customer database* has been selected in the database combo box.

Selecting this option starts the browser - **in delete mode**. The database can be browsed and the selected structure can be deleted.

Button

4.4.7 Task Start (or Name)

All searches must be started from the Commander. A query must have been formulated and be present in either the structure panel, or the fact panel, or both. After starting, a dialog box displays the status of the search, and the Search button changes to a Stop button to stop the search. When the search is completed, a dialog box displays the hit list number and number of hits, and asks if the hit list should be displayed or not.

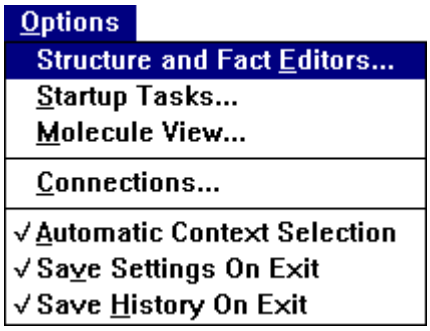
If Autonom is the active application this option will start the Autonom program which will generate a name for the current structure.

Shortcut: F7

Button

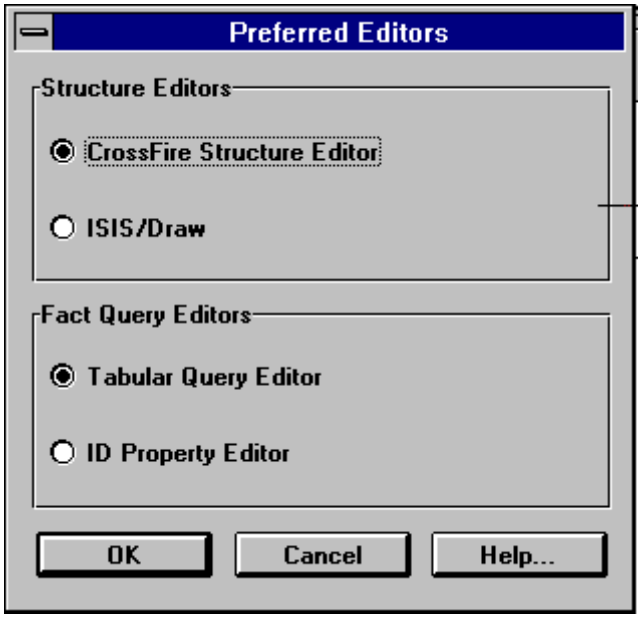
4.5 Options menu commands

The Options menu offers the following commands:



4.5.1 Structure and Fact Editors

Choose this option to display the Preferred Editor dialog box.



You can select which Structure Editor and Fact Editor you would like to use.

⌘ Macintosh

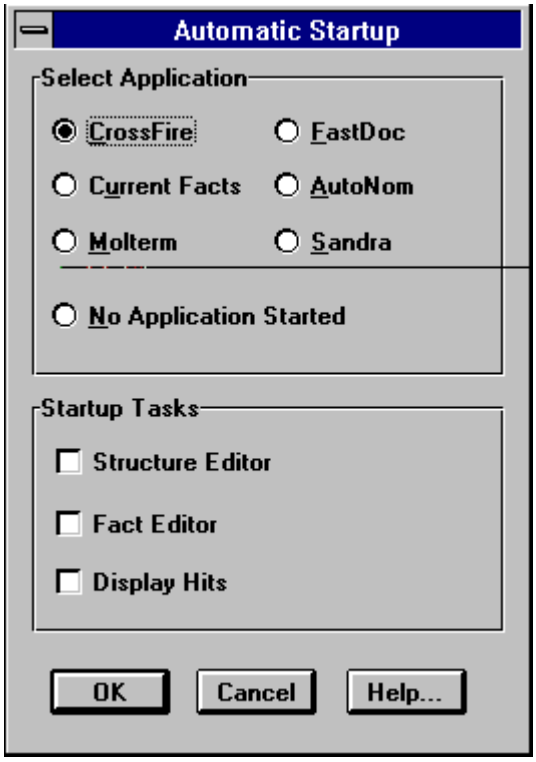
Currently, only the native CrossFire Structure Editor is available.

4.5.2 Automatic Context Selection

Switch this option on, to automatically have the display context be changed to match the query. For example, if you search for a reaction, the automatic display context will also be reaction.

4.5.3 Startup Task (Options menu)

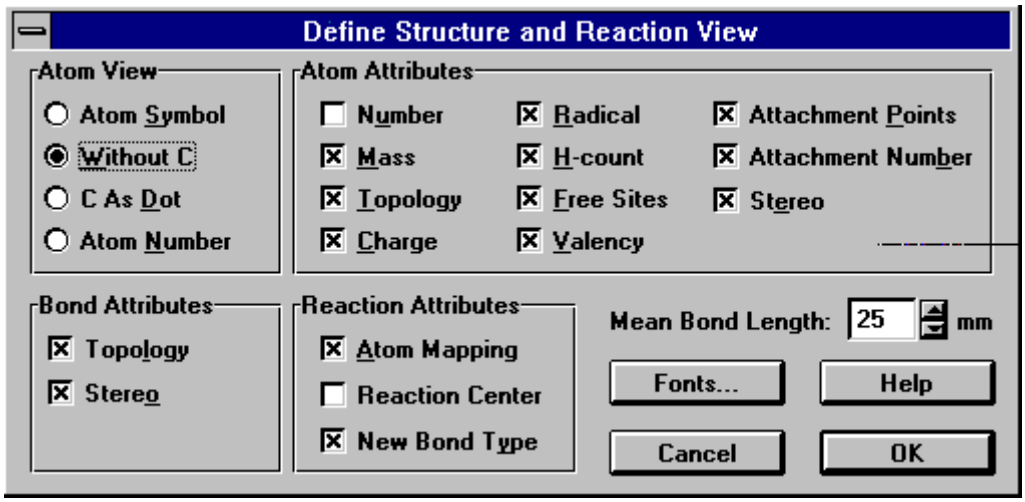
Choose this option to display the Startup Task dialog where you can select your start-up application and task.



Setting the startup application to CrossFire, means that after starting the Commander the Login procedure for CrossFire will be automatically started.

4.5.4 Molecule View

Choose this option to display the Molecule View Dialog where you can set the display attributes for atoms, bonds and reactions.



Atom View

Choose one of the following options:

Atom Symbol	Includes C for carbon
Without C	Suppresses the display of C
C as dot	Displays a dot for the carbon atoms
Atom Number	Displays the number of the atom

Atom attributes

Switch the following options on or off as required:

Number	Displays the number of the atom in the structure
Mass	Displays the abnormal mass if present.
Topology	Displays topology if non-default.
Charge	Display the charge if non-default.
Radical	Displays the radicals if non-default.
H-count	Displays min. and max. H-counts if present.
Free Sites	Displays the free sites if present.
Valency	Displays the valency if non-default.
Attachment Points	Displays the attachment points of generic residues.
Attachment Number	Displays the attachment numbers of atoms in the parent structure.

Bond Attributes

Switch the following attributes on or off as required:

Topology	Displays the topology if non-default.
Stereo	Displays stereo-specific bond attributes if present.

Mean Bond Length

Set the mean bond length by pressing the button to display the mean bond length dialog box.

Either enter the number directly or use the micro-scrolls to increase decrease the current value.

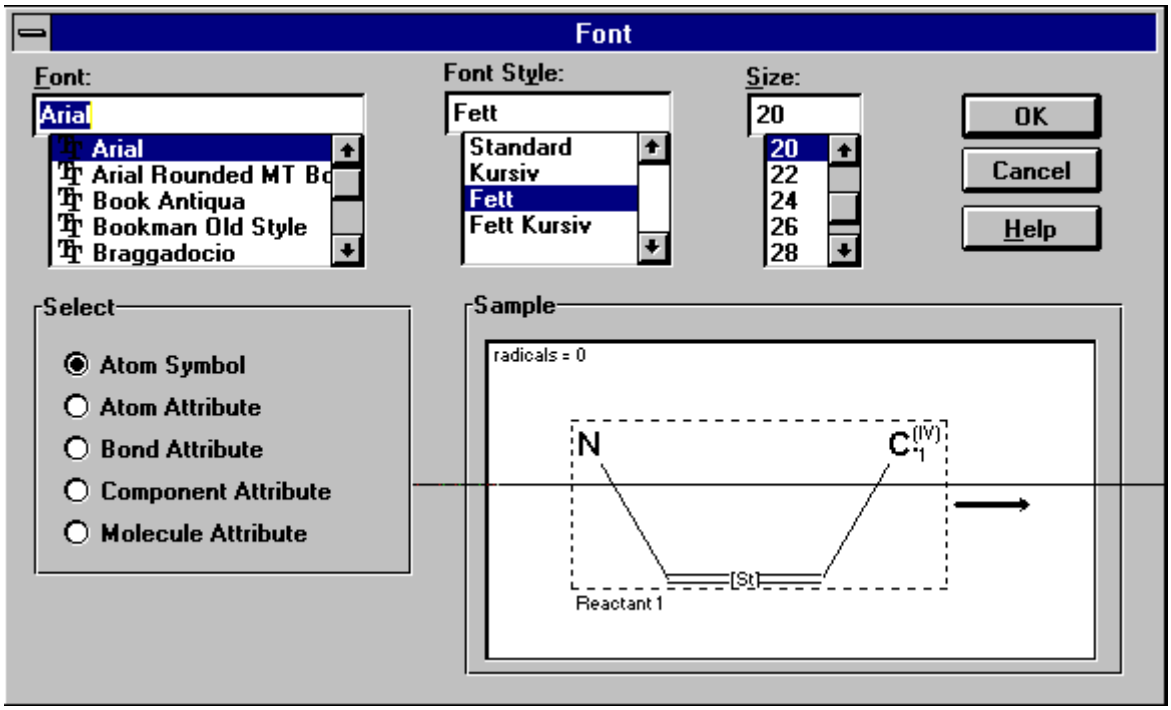
Reaction Attributes

Switch the following attributes on or off as required:

Atom Mapping	Displays the atom mapping if present.
Mapping Number	Displays the mapping number if present.
New Bond Type	Displays the new bond type if present.

Fonts

Press this button to call up the font selection box.



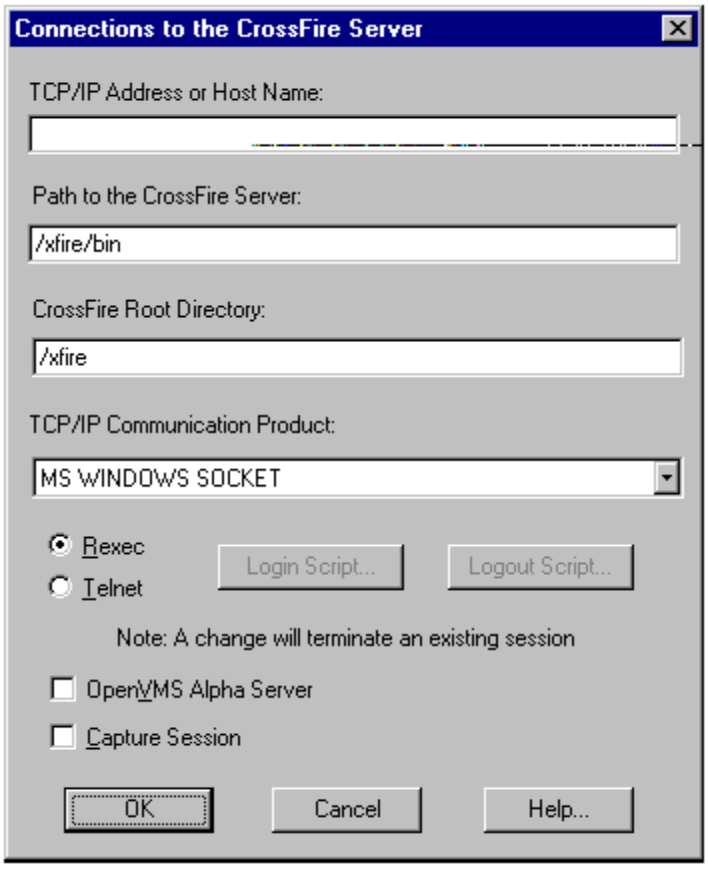
This dialog box allows you to set the fonts for molecule display. You can independently set the following:

Atom Symbol
Atom Attribute
Bond Attribute
Component Attribute
Molecule Attribute

The Sample window will reflect the changes as you make them.

4.5.5 Connections

Choose this option to display the Connections dialog where you can enter your connection parameters.



Enter the connection parameters in this dialog box for connection to the CrossFire server.

The entries will normally have been correctly input by the network supervisor. If you change any entry you might loose the connection to the server and CrossFire will not run.

The following must be input:

TCP/IP address or host name

Here you can enter a numeric address (e.g. 111.111.111.001) or a symbolic name (e.g. test.com).

Path to the CrossFire server

Please ask your system administrator for more details. If you have a default installation on the server, then the entry should be /xfire/bin for an RS6000 (AIX), and @xfbin: for a DEC Alpha server (OpenVMS). The entry for the DEC Alpha

server will be set automatically if the box labeled OpenVMS Alpha Server is checked.

CrossFire root directory

Please ask your system administrator for more details. If you have a default installation on the server, then the entry should be /xfire for an RS6000 (AIX), and for a DEC Alpha machine (OpenVMS).

TCP/IP communications product

The Beilstein Commander (Windows Version) is able to work with Novell LAN Workplace 4.0/4.1 or any TCP/IP product that supports Microsofts Windows Socket version 1.1.

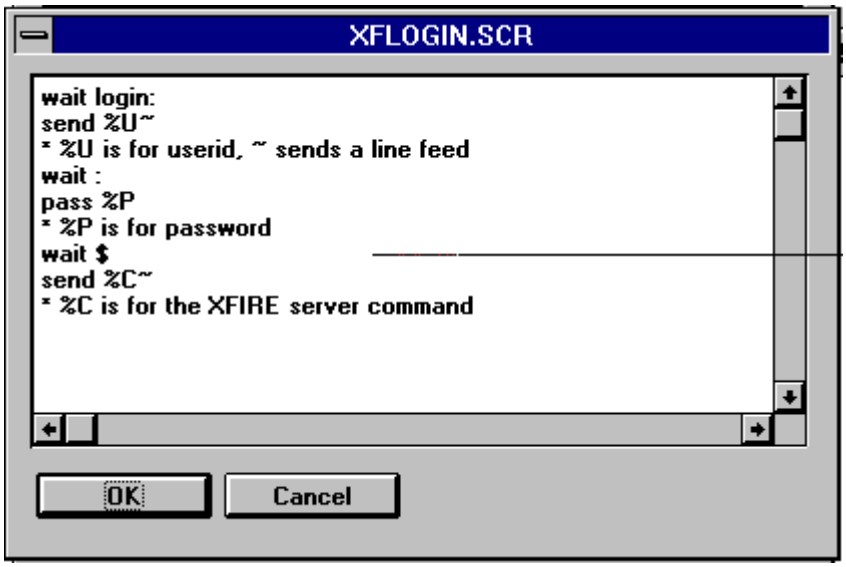
The Beilstein Commander (Macintosh Version) supports MacTCP or compatible TCP/IP products.

REXEC or TELNET service

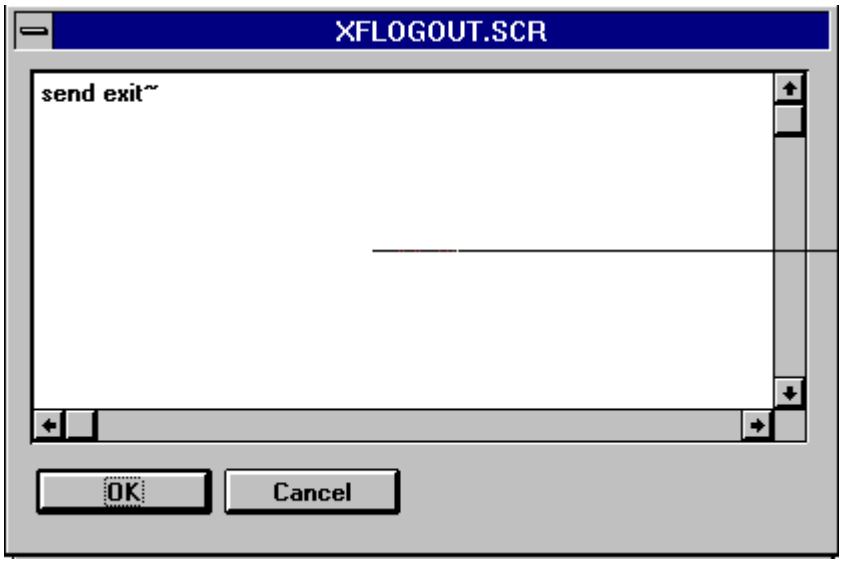
The two radio buttons allow you to choose between REXEC and Telnet. Please ask your system administrator for more details. Usually Telnet services are used to connect to the server. If you enable Telnet then you might have to edit Login and Logout script files. You can click on the appropriate buttons and you will get a dialog box which allows you to modify the default script files. These are standard ASCII files located in the Windows directory or, for Macintosh, in the Beilstein Commander program directory. They can be edited with typical ASCII editors in the Windows environment. Macintosh users should not edit them with any Macintosh text editor, but within the edit box of the Commander.

For a Telnet session, you will require a Login Script, and example is as follows:

Login Script



Logout Script



OpenVMS Alpha Server

If this checkbox is enabled the Beilstein Commander can communicate with a DEC Alpha server running under OpenVMS. It will also change the entry for “Path to the CrossFire server”. Please do not enable it if you are using a different server.

Capture Session

If this checkbox is enabled, CrossLink will write a capture file MB.DMP into the Beilstein Commander working directory containing all communication (input and output) which has been exchanged between client (Beilstein Commander) and

server. The content is a mixture of HEX and ASCII characters and should be used if you need help from the Beilstein HelpDesk, so that our team can analyze any communication problem.

4.5.6 Save settings on Exit

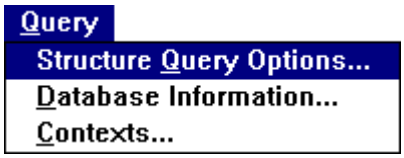
When this option is active user defined settings will be saved and used again in the next session.

4.5.7 Save History on Exit

When this option is active the session history will be saved and be available again in the next session.

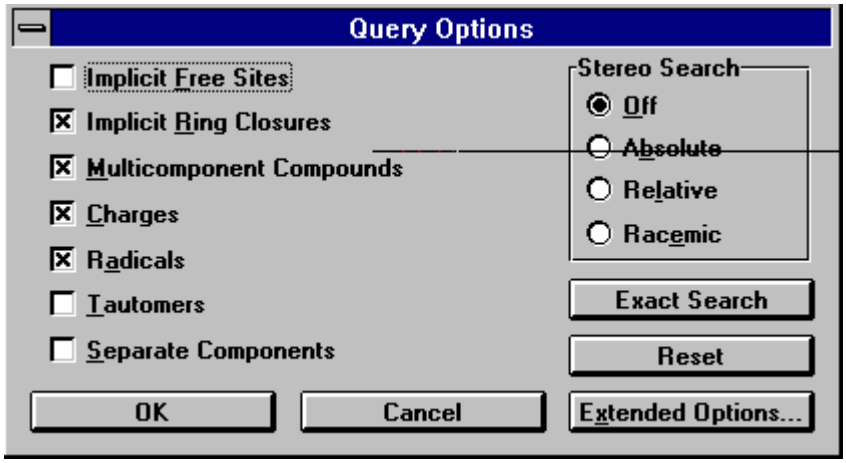
4.6 Query menu commands

The Query menu offers the following commands:



4.6.1 Structure Query Options

Selecting this menu item causes the query option dialog box to be displayed.



Options can then be set. Pressing OK closes the dialog box, the selected options are then displayed as a string in the options window. If the options button is pressed when options have already been set, these settings will be displayed in the dialog box.

Shortcut: use the query options buttor

The following global options can be set for the search. These override all analogous atom attributes; for example, setting free sites on all atoms in this dialog box overrides any free site atom attribute information set when drawing the query.

Use the reset button to go back to the system default values.

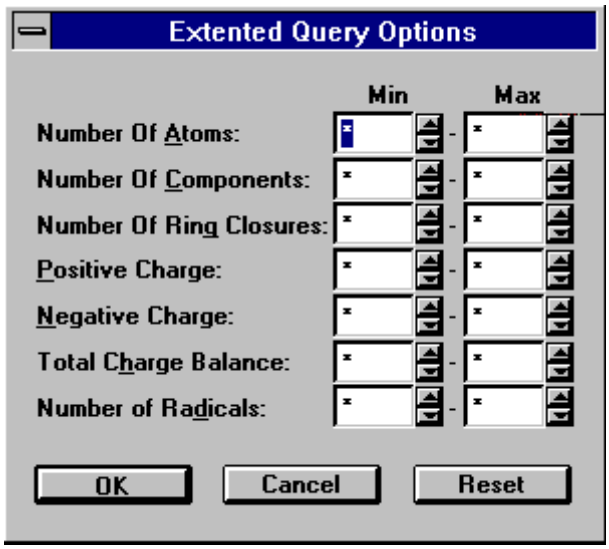
Implicit Free Sites	Sets maximum free sites, up to the maximum allowed valency on all atoms.	Default - Off
Implicit Ring Closures	Allows or excludes ring closures between atoms or groups with free sites.	Default - On (Allowed)

Multicomponent Compounds	Allows or excludes multicomponent structures.	Default - On (Allowed)
Charges	Allows or excludes charges other than those explicitly drawn.	Default - On (Allowed)
Radicals	Allows or excludes radicals other than those explicitly drawn.	Default - On (Allowed)
Tautomers	Switches the tautomer search on. See section on tautomer searching for more information.	Default - Off.
Separate Components	When more than one isolated component is drawn in the query, this switch defines whether they are to be retrieved in the same component or in different components in the hit.	Default - Off (Separate)
Stereo Search	Choose between: Off, Absolute, Relative and Racemic. See section on stereo searching for more information	Default - Off.

The **Exact Search** button sets the query options to exclude all multicomponent, charged or radical compounds.

4.6.2 Structure Search Restrictions

The Extended Options allow the following global restrictions can be set for the search.



Minimum and maximum values can be independently set using the micro-scrolls. Use the reset button to go back to the system default values (no restrictions).

Number of Atoms The total number of atoms to be found in the retrieved structure.

Number of Components The total number of components to be found in the retrieved structure. (Salts and addition compounds).

Number of Ring Closures The total number of rings to be found in the retrieved structure. (Defined as the smallest number of ring bonds which must be broken in order to convert the structure into an acyclic structure).

Positive Charge The total number of positive charges to be found in the retrieved structure.

Negative Charge The total number of negative charges to be found in the retrieved structure.

Total Charge Balance The total charge balance to be found in the retrieved structure.

Number of Radicals The total number of radicals to be found in the retrieved structure.

4.6.3 Stereo Searching

This can be carried out for full-structures, generic structures and Markush structures.

The structure editor allows two types of stereochemistry to be defined for molecules. Firstly the absolute configuration of asymmetric or chiral centers can be defined by using bond types of steric-up or steric-down or steric unknown. Direct input of R, S configuration according to the Cahn-Ingold-Prelog conventions in not possible.

Secondly, configuration of double bonds can be specified by using the bond type of “double stereo.” When this descriptor is used, the absolute input configuration will be searched for in the database. Direct input or E, Z or Syn/Anti descriptors is currently not possible.

Absolute Stereo Search

When this level is used the exact configuration will be searched for. Only compounds which have the identical absolute configuration as the query structure will be found as hits.

Relative Stereo Search

The same as for Absolute, but also retrieves the mirror image and the racemate of the query. Thus, structures will be retrieved with all stereocenters as defined in the query, and also those with all their stereocenters of opposite configuration to the definition in the query. This way, compounds and their enantiomers can be retrieved.

However, no diastereoisomers will be retrieved.

Racemic Stereo Search

Retrieves only the racemate of the query.

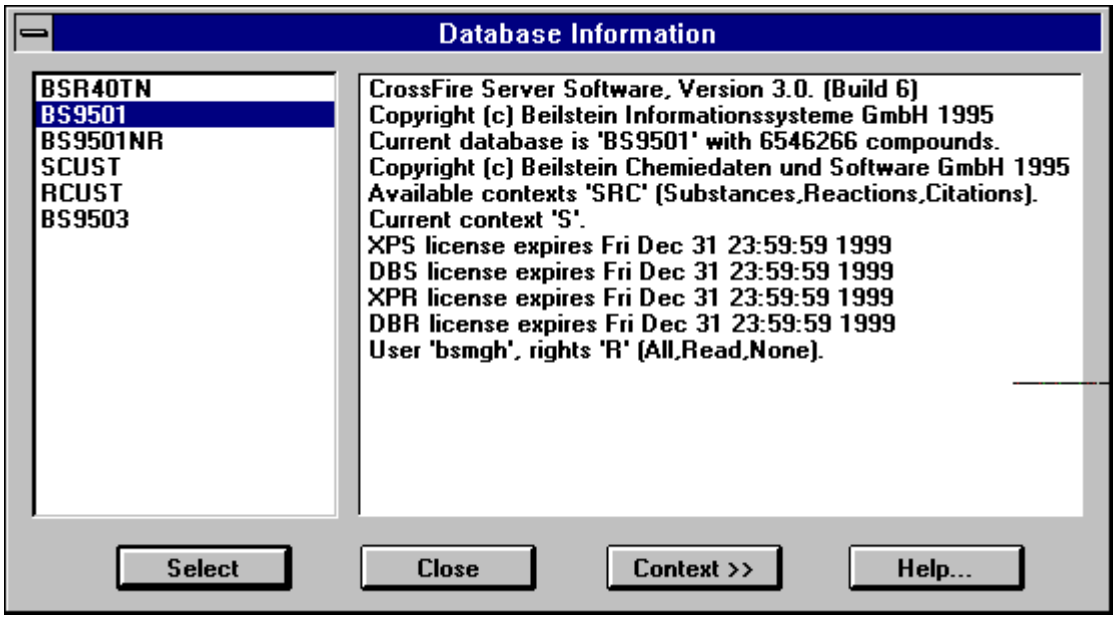
4.6.4 Tautomer Searching

A compound which exhibits prototropic tautomerism is one which exists in two or more forms, arrived at by a formal transfer of a hydrogen atom to (or from) a heteroatom from (or to) any other atom in the compound, accompanied by a rearrangement of electrons which results in one, or more of the double bonds being shifted.

This type of search is only valid for full structures.

4.6.5 Databases

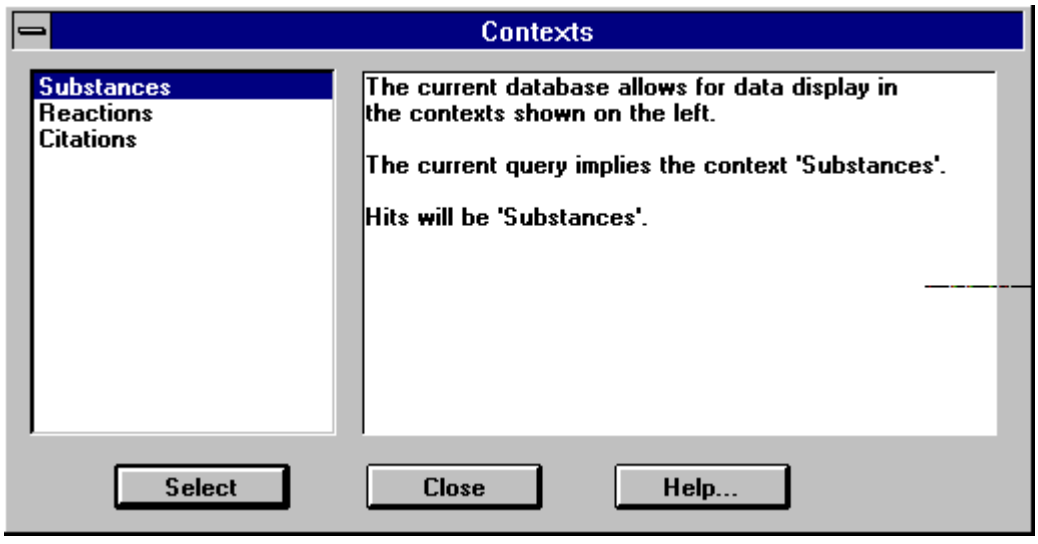
Use this option to display the Databases dialog box where you can choose the database to search. When using CrossFire, you can choose between searching the Beilstein File and any CrossFire customer databases that you may have. Only one database may be selected at a time.



Shortcut: Use the database selection box

4.6.6 Display Context

This option will only be enabled when the Beilstein File has been selected in the database combo box.



shortcut use the display as context selection box.

This box contains a list of the available display contexts.

Choose between:

substance

reaction

By default, the display context is the same as the query context. Thus, a hitlist retrieved from a substance query (molecule or property) will be displayed as a list of molecules and their properties. You can change the display context either before you start the search, or you can convert a hit list and display it in a different context. For example, you can take a list of reactions and display these records as a list of citations.

The display context can also be changed on-the-fly for individual records. This is achieved by means of hyperlinks. There are now three distinct types of hyperlinks: Substance (using the Beilstein Registry Number), Reaction (using the Reaction Identification Number) and Citation (using the citation Identification Number). Irrespective of how you are displaying information, these links permit instant access to information about other substances, reactions or citations.

4.7 Help menu commands

The Help menu offers the following commands, which provide you assistance with this application:

Contents	Offers you a table of contents of topics in the help system.
Using Help	Provides general instructions on using help.
About	Displays the version number of this application.

4.7.1 Contents command

Use this command to display the Help opening screen . From the opening screen, you can jump to step-by-step instructions for using the Beilstein Commander and various types of reference information.

Once you open Help, you can click the Contents button whenever you want to return to the opening screen.

4.7.2 Using Help command

Use this command for instructions about using Help.

4.7.3 About command

Use this command to display the copyright notice and version number of your copy of the Beilstein Commander.

4.7.4 Context Help command

Use the Context Help command to obtain help on some portion of the Beilstein Commander. When you choose the Toolbar's Context Help button, the mouse pointer will change to an arrow and question mark. Then click somewhere in the Beilstein Commander window, such as another Toolbar button. The Help topic will be shown for the item you clicked.

Shortcut

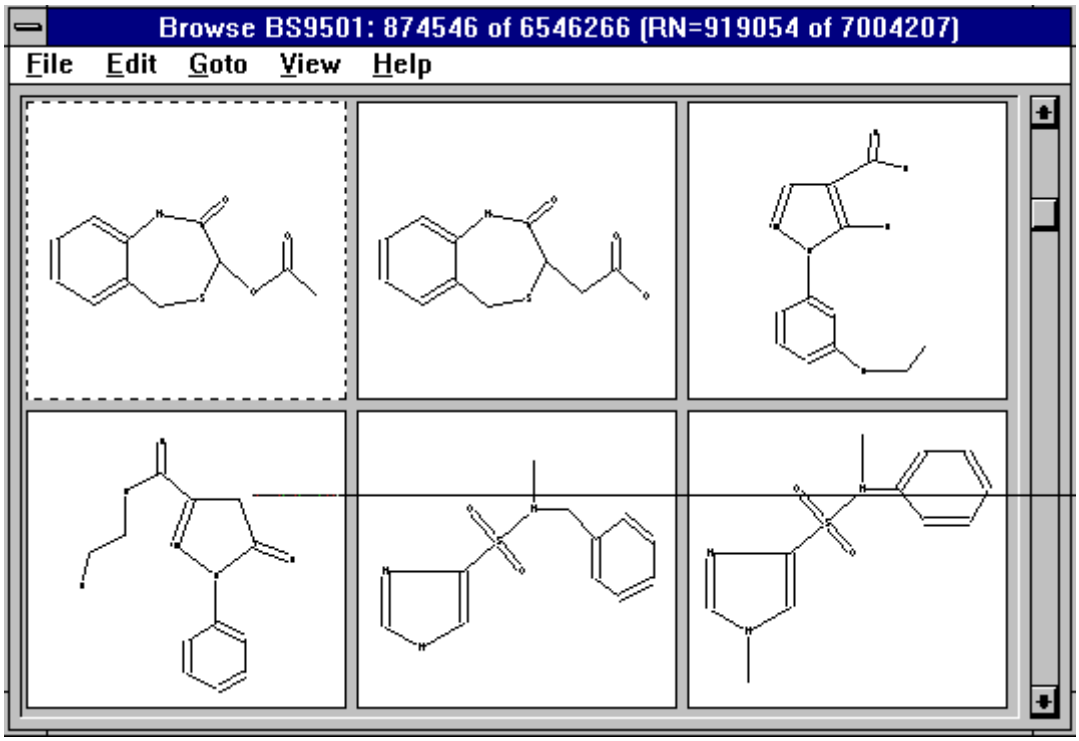
Keys: SHIFT+F1

The Browser

5

5. The Browser

The Browser is used either when examining *.BSD files of factual queries, structure queries or templates, or when viewing the History, hitsets or structures in a database.



The Browser has a menu bar and a configurable number of cells for viewing the entries in the files or lists.

5.1 The File Menu

The file menu has the following options:

5.1.1 Load

This option is active for the following:

- History
- Hitsets
- Structures
- Fact Queries
- Databases

Use this option to load the selected entry into the active application.

5.1.2 Save

This option is only active for customer files or databases. Use it to save the structure in the Beilstein Commander, in the selected place in the customer database.

5.1.3 Delete

This option is only active for customer databases. Use it to delete the selected entry from the customer database.

5.1.4 Exit

Exit the Browser and return to the calling application.

5.2 The Edit Menu

The edit menu has the following option:

5.2.1 Copy

Copies the selected entry to the clipboard.

5.3 The Goto Menu

The Goto menu has the following options:

5.3.1 First User Item

This option is only active for customer files or databases. Use this Goto function to find the first item in your own section of a customer database.

5.3.2 Last User Item

This option is only active for customer files or databases. Use this Goto function to find the first item in your own section of a customer database.

First Gap

This Goto option finds the first gap in a file or customer database where you will be able to store a structure.

5.3.3 Enter Item No.

This Goto option allows you to find a particular entry in the database. Enter the sequential number in the edit field.

5.3.4 Enter Reg. No.

This Goto option allows you to find a particular entry in the database. Enter the registry number in the edit field.

5.3.5 First Used Item

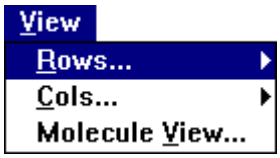
This Goto option finds the first entry in the file or database.

5.3.6 Last Used Item

This Goto option finds the last entry in the file or database.

5.4 The View Menu

The view menu has the following options:



5.4.1 Rows

Use this option to set the number of rows displayed in the Browser.

5.4.2 Cols.

Use this option to set the number of columns displayed in the Browser.

5.4.3 Molecule View

The molecule view dialog box allows you to define how you would like the molecules to be displayed.

See section on molecule view for more information.

5.5 The Help Menu

5.5.1 Contents

Use this command to display the Help opening screen . From the opening screen, you can jump to step-by-step instructions for using the Display and various types of reference information.

Once you open Help, you can click the Contents button whenever you want to return to the opening screen.

6

6. Appendices

6.1 Appendix A - Other Applications From Beilstein Information

6.1.1 Application: Current Facts

Current Facts in Chemistry is a collection of the latest information on organic and medicinal chemistry delivered four times a year on CD-ROM.

With Current Facts, every quarter, investigators have access to the most recent twelve months of organic chemistry as reported in 100 top journals. Literature, structures, reactions, preparations, physical and chemical properties including toxicological and environmental data, keywords, citations, authors and CODENs. Scientists needing access to the most recent advances in their field, find in Current Facts an indispensable tool for daily research

Using Current Facts you can search for structures, substructures, stereoisomers and tautomers of compounds presently under investigation.

Substructure query types can include bond and stereo-chemical descriptors, atom types, generic groups (e.g. acyclics, hetero-cycles, etc.).

The fact editor is a sophisticated data navigator that allows posing elaborate queries with remarkable ease. Boolean operators (and, or, not) enable the scientist to combine queries, and to manipulate lists of hitsets.

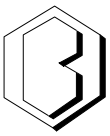
Current Facts displays structures, and as many data fields as the user wishes to see. Hypertext links let you jump directly to the record of the highlighted compound. You can use this to navigate along synthesis paths.

6.1.2 Application: Molterm

MOLTERM is an ASCII terminal-emulation program with an integrated structure and fact editor running under Microsoft Windows. Having a mouse-supported structure editor allows construction of detailed full- and substructure searches and translation into the structure commands of STN, DIALOG and DARC. Since MOLTERM is a Windows program it can exchange files and data with other Beilstein programs via the clipboard, in addition MDL's Molfile format is also supported (MDL Information Systems).

The most important component is the fact editor. Without a detailed knowledge of the field names, you can prepare a complex factual search in tabular form. MOLTERM then translates the table into the retrieval language of the appropriate host (STN or DIALOG). No other communication program is able to construct, so clearly, complex queries for chemical databases.

Beilstein Online - access to factual data for organic compounds on STN and Dialog



In the area of organic chemistry Beilstein Online is the world's largest factual database. With about 7 million heterocyclic, acyclic and isocyclic compounds, the Beilstein database covers the literature from 1779 to the present.

The contents and data structure are based on the Beilstein Handbook of Organic Chemistry. The online file contains Beilstein handbook data from the Basic Series to Supplement IV, covering the literature from 1779 to 1959, and structures and facts which have been abstracted from the primary literature. Regular updates give you access to the latest information published in the chemical literature. The file is available on the hosts STN and Dialog.

Beilstein Online offers a variety of search options which make this electronic information system an excellent reference tool for organic chemists and information specialists. You can either search for structures, facts, bibliographic information or perform combined searches.

Identify substances via the

- Beilstein Registry Number
- CAS Registry Number
- Substance name
- Molecular formula
- Structure diagram

etc.

Find information on chemical data for

- Preparations
- Reactions
- Isolation from natural product
- Chemical derivatives

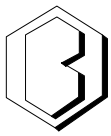
Get physical property data such as

- Optical Data
- Mechanical properties
- Multicomponent system data
- Spectral properties
- Thermodynamic properties

etc.

Physiological behaviour offers information on

- Biological function,
- ecological data



- toxicity and the
- use of a compound

Get bibliographic information on e.g.

- Author,
- journal title,
- CODENs,
- patents or
- publication year

6.1.3 Application: Autonom

IF YOU CAN DRAW IT, IF YOU CAN SYNTHESIZE IT, AUTONOM 2.0 CAN NAME IT

Chemists engaged in organic synthesis spend a significant amount of their time assigning systematic names to compounds. Systematic chemical nomenclature is a set of rules, proposed by IUPAC, by which chemists communicate information about the compounds they have developed.

The IUPAC rules for assigning systematic names to chemical structures are complex and frequently lead to ambiguous names. These difficulties can be overcome by algorithms which analyze the structural diagram of the compound and generate the systematic name automatically.

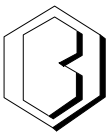
AUTONOM (AUTOmatic NOMenclature) release 2.0 is a windows-based program (for the PC and Macintosh) which generates IUPAC names from graphic structures.

The algorithms in AUTONOM 2.0 name your structure in the same way a nomenclature specialist would: first AUTONOM identifies the parent fragment of a structure by applying the appropriate IUPAC nomenclature principles, it then orders the other structure fragments according to the predefined nomenclature hierarchy. Next, all recognized fragments of the input structure (ring systems, chains, functional groups) are related to their corresponding name fragments and finally assembled to from a complete, IUPAC-compatible name.

AUTONOM 2.0 uses the Beilstein structure editor; however, it can be configured to use any editor that supports MDLs sketch file format as input.

NEW FOR RELEASE 2.0

Two-component structures are now handled (previous version was limited to naming single component substances) including inorganic cations, anions and inorganic neutral species.



Organic cyanamide derivatives

Organic carbodiimide derivatives

(Carbox)amidines

Hydroxamic acid derivatives

Phthalocyanine derivatives

Alternating silicon and hetero atom chains

Greatly enhanced dictionary of trivial annelated ring systems

ADVANTAGES OF AUTONOM 2.0

AUTONOM delivers IUPAC compatible names in seconds

AUTONOM creates names based on algorithms

AUTONOM will not name a structure incorrectly: It gives a warning if the structure cannot be named

AUTONOM's success rate is up to 86% of its applications

AUTONOM works with a library of more than 7,000 entries in the ring dictionary

AUTONOM recognizes abnormal valences

AUTONOM can name single charged compounds

AUTONOM has a large database of functional groups

6.1.4 Application: Sandra

SANDRA - your window to the Beilstein Handbook

Presently, the Beilstein Handbook contains carefully checked information on over 3.0 million organic compounds. Without SANDRA, locating information on any particular compound in the Handbook requires some knowledge of the Beilstein classification system and an appropriate search technique. SANDRA relieves you of this burden and is easy to use. You simply draw structural formulas, using a mouse. These are then entered via a fast, flexible graphic input system and analyzed by SANDRA which then tells you where to look for your compound (or its analogues) in the Beilstein Handbook, assuming the structure exists. Hardware Requirements: IBM PC compatible personal computer with at least 256k memory, IBM and Hercules graphics card, Microsoft or compatible mouse; a screen dump can be made with IBM-compatible printers.

The Beilstein Handbook of Organic Chemistry , commonly referred to as "Beilstein", contains important information published since 1779 about the manufacture and properties of carbon compounds. With over 500 single volumes

the Beilstein Handbook today constitutes the world's largest collection of critically evaluated organic compounds in printed form.

The Handbook is published in series, each covering the literature of a certain time period. All volumes from the Fifth Supplement (EV) onwards are published in English. Each series consists of 27 (nominal) volumes, which may be subdivided into several subvolumes in the more recent series. The individual compounds are arranged according to the Beilstein System which classifies all organic compounds according to their structures.

For each compound described, Beilstein covers the following aspects :

* structural formula
* compound name(s)
* molecular formula
* constitution and configuration
* natural occurrence
* isolation from natural products
* preparation and purification
* structural and energy parameters of the molecule
* physical properties
* chemical properties (reactions)
* characterization and analysis
* salts and addition compounds.

Altogether more than 350 different kinds of physical data are found in the Handbook. For anyone concerned with organic chemistry, the Beilstein Handbook is a unique and indispensable source of information.

In 1981 *Beilsteins Handbuch der Organischen Chemie* celebrated its centenary: The first edition of Beilstein appeared in the years 1881-1883 as two subvolumes, in which around 15,000 carbon compounds were described on 2,200 pages. Evaluation of the literature and editorial treatment for this first edition, and the two subsequent editions which rapidly followed, was managed single-handedly by *F. K. Beilstein*, whose name was given to the Handbook and the Company.

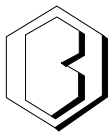
F. K. Beilstein was born the son of German parents in St. Petersburg in 1838; after studying chemistry in Heidelberg, Munich and Göttingen, he was named to the Chair of Chemistry at the Imperial Technology Institute in St. Petersburg, where he succeeded Mendeleev. His plans to publish a handbook of organic

chemistry rapidly matured, a task which was to occupy him fully for 40 years, until his death in 1906.

The immense success of the 1st edition of his handbook soon compelled him to publish a 2nd edition, which appeared in the years 1885-1889 and extended to three volumes with 4,080 pages. Between 1892 and 1906 the third edition appeared, together with a supplementary series and a complete index for the 3rd edition. These 8 volumes, including the supplementary series, contained critically reviewed material on all the carbon compounds then known, in around 11,000 pages.

Even before work had been completed on the 3rd edition, Beilstein realized that publication of a handbook of this type exceeded the working capacity of any one individual. He thus handed over the work of further publication to the German Chemical Society, which, under the editorship of P. Jacobson and B. Prager, started with the publication of the 4th edition in 1918. In 1933, F. Richter took over the editorship, followed by Hans-G. Boit, who was publisher of the handbook and director of the Beilstein Institute in Frankfurt am Main from 1961 until March 31st, 1978. Since April 1st, 1978, Reiner Luckenbach has been director of the Institute.

The “Beilstein-Institut”, which adopted the legal status of a trust in 1951, is engaged in close cooperation with Beilstein-Informationssysteme GmbH in the rapid publication of the supplementary series of Beilstein.



6.2 Appendix B - CrossFire Client Script Commands

The CrossFire Client uses two script files to establish or terminate TELNET sessions:

- XFLOGIN.SCR
- XFLOGOUT.SCR

Both scripts are ASCII text files with the following rules:

- Lines starting with one of several 4-letter-keywords plus a blank are interpreted as commands. All other lines are comments. In a command line, the characters from 6 up to excluding the line feed are a single command parameter.
- Keywords are case-insensitive, the case of command parameters is not changed.

The following commands are defined:

Command	Meaning
WAIT ”string“	Wait until the host sends ”string“.
SEND ”string“	Send ”string“ to the host. If a carriage return keystroke is to follow the characters sent, a tilde (~) has to be the final character of ”string“.
PASS ”password“	Send a password (suppressing screen output). A tilde (see SEND) should not be appended. Instead of inserting a password into the script, you should consider using the %P place holder.
DELA ”delay time“	Wait for ”delay time“ seconds.

Within the script, you may use the following place holders to represent fields from the ”Login to Server“ and ”Options - Connections“ dialog boxes:

Place holder	Meaning
%U	User ID from the Login dialog box.
%P	Password from the Login dialog box.
%C	Command to start the CrossFire Server. This command is constructed from the CrossFire program path and the

	database root path in the Options - Connections dialog box.

Example 1, typical procedure

wait login:

send %U~

*~ sends a line feed

wait :

pass %P

wait $

send %C~

Example 2, a firewallin-between:

wait >

* > is the Firewall prompt

send c 123.456.789.101

*this is the connect command for accessing an external server

wait login:

send %U~

* %U is for userid, ~ sends a line feed

wait :

pass %P

* %P is for password

wait $

send %C~

* %C is for the XFIRE server command

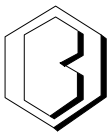
6.3 Appendix C - BSD (Rosdal) / MDL Sketch format conversion

6.3.1 Conversion of MDL Sketch format to BSD

Since in the native CrossFire structure editor, the basic philosophy is that the default setting for free sites is none, this will also be assumed for structures coming from ISIS/draw. Thus to set maximum free sites on particular atoms, this must be explicitly done from within ISIS/Draw. To set free site on all atoms, this is most easily done using the Structure Query Options in the Commander.

All attributes can be converted with the following exceptions:

1. R logic is not supported and is ignored.
2. Link nodes will be ignored. Resolve link node using R-groups.
3. Amino acid symbols are not supported and are translated into G groups.
4. Atom aliases are ignored.
5. Unsaturated atoms are not supported.
6. Atom value is not supported.
7. Ring bond count is not supported.
8. No of R group in Atom is not supported.
9. Singlet diradical is not supported.
10. Aromatic bonds are not supported.
11. Bond stereo care is not supported.
12. Mappings more than 1 is not supported.
13. Mappings no partner is not supported.
14. Atom exact change is not supported.



6.3.2 Conversion Rosdal to MDL Sketch format

All attributes can be converted with the following exceptions:

1) Predefined atom list M.
2) Atom symbols; Ku, Ha, or Rf.
3) Shortcuts or predefined generic group symbols.
4) AC when the definition is due to a H atom bond being broken.

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